OPTIMIZATION ON ACRYLIC ACID PLANT BY USING ASPEN PLUS

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Thesis submitted in partial fulfillment of the requirements for the award of the degree of Bachelor of Chemical Engineering

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SUPERVISOR'S DECLARATION

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

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STUDENT'S DECLARATION

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

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Special Dedication to my supervisor, my family members,
my friends, my fellow colleague and all faculty members
for all your care, support and believe in me.

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

PROPY-01	–	Propylene
NITRO-01	–	Nitrogen
OXYGE-01	–	Oxygen
CARBO-01	–	Carbon Dioxide
WATER	–	Water
ACETI-01	–	Acetic Acid
ACRYL-01	–	Acrylic Acid
DIISO-01	–	Diisopropyl Ether
PROIN	–	Inlet of Propylene
PROOUT	–	Outlet of Propylene
ACRY	–	Mole Flow of Acrylic Acid
TACRY	–	Total Mole Flow of Acrylic Acid
ACET	–	Mole Flow of Acetic Acid
TACET	–	Total Mole of Acetic Acid
DIPE	–	Diisopropyl Ether
DIISO	–	Mole Flow of Diisopropyl Ether
TDIISO	–	Total Mole Flow of Diisopropyl Ether
TOTAL 1	–	Total Mole Flow of Stream 22
TOTAL 2	–	Total Mole Flow of Stream 21
T	–	Temperature
P	–	Pressure
WAT	–	Water
FS	–	Feed Stages Location
RR	–	Reflux Ratio
RD	–	Re-boiler Heat Duty
DIAM	–	Diameter
LENGTH	–	Length
PD	–	Pressure Drop

TUBE	–	Number of Tube
TEM	–	Temperature
Pres	–	Pressure
CD	–	Condenser Heat Duty
NS	–	Number of Stage
BR	–	Bottom Rate
CT	–	Constant Temperature
CP	–	Constant Pressure
REACRY	–	Recovery of Acrylic Acid
REACET	–	Recovery of Acetic Acid
PUR 1	–	Purity of Acrylic Acid
PUR 2	–	Purity of Acetic Acid

PENGOPTIMUMAN PADA LOJI ASID AKRILIK DENGAN MENGGUNAKAN ASPEN PLUS

ABSTRAK

Pengoptimuman pada reacktor dan pemisah bahagian daripada loji asid akrilik telah diyiasatkan dalam pengajian ini. Untuk mendapatkan kadar pengeluaran yang lebih tinggi dan kualiti yang lebih baik bagi produk asid akrilik, Aspen Plus telah diggunakan untuk mensimulasikan dan mengoptimumkan loji asid akrilik tersebut. Unit operasi yang dilibatkan adalah reacktor system, wap pemulihan system dan pemulihan system cecair. Metodologi penyelidikan ini telah dipisahkan kepada tiga fasa, iaitu, pertama sekali mensimulasikan loji asid akrilik dalam keadaan yang mantap, kedua analisis sensitiviti, dan akhirnya adalah pengoptimuman. Berdasarkan keputusan yang telah dapat, loji asik akrilik telah berjaya mensimulasikan dalam Aspen Plus dan kadar pengeluaran akhir produk adalah diterimakan. Untuk bahagian yang pengoptimuman, suhu optimum reacktor adalah 315℃ untuk mendapatkan hasil maksimum asid akrilik, iaitu 0.77254. Untuk unit dram flash, optimum suhu dan tekanan adalah 25℃ and 4.84atm masing-masing. Untuk menara penyerapan dan cecair-cecair pemerah, optimum kadar aliran air dan pelarut adalah 100kmol/j dan 1350kmol/j masing-masing untuk mendapatkan lebih daripada 99% asid akrilik dan asid asetik. Untuk turus penyulingan kesatu, peringkat suapan lokasi optimum, nisbah refluks dan duti haba dibekalkan adalah nombor 8, 4.44308 dan 180000MJ/j masing-masing untuk memaksimumkan pemulihan asid dan pelarut. Untuk turus penyulingan kedua, peringkat suapan lokasi, nisbah refluks dan duti haba dibekalkan adalah nombor 23, 10.5 dan 3000MJ/j masing-masing untuk mendapatkan kesucian asid akrilik yang paling tinggi. Untuk keputusan keseluruhan, ia mendapati bahawa mengoptimumkan keadaan operasi unit akan mendapatkan produk yang berkualiti dan lebih banyak bahan boleh dipulihkan.

OPTIMIZATION ON ACRYLIC ACID PLANT BY USING ASPEN PLUS

ABSTRACT

In this research of study, optimization of reactor and separators sections on acrylic acid production plant was investigated. In order to obtain higher production rate and maintain desired quality of products, the Aspen Plus simulator is used to simulate and optimize on the acrylic acid plant. The units proceed with optimization consists of reactor system, vapour recovery system (adsorption tower, and flash drum) and liquid recovery system (liquid-liquid extractor, and distillation column). The research methodology as separated into three phases, which are steady state simulation, sensitivity analysis and optimization. Based on the result obtained, the acrylic acid production plant was simulated successfully in Aspen Plus flow sheet and the final production rate of products is acceptable. For the optimization, optimum temperature of reactor is 315℃ in order to obtain the maximum yield of acrylic acid which is 0.77254. For the flash drum unit, optimum temperature and pressure are 25℃ and 4.84atm respectively. For the absorption tower and liquid-liquid extractor, optimum molar flow rate of water and solvent are 100kmol/h and 1350kmol/h respectively in order to recover more than 99% of acrylic and acetic acid. For the distillation column 1, optimum feed stages location, reflux ratio and re-boiler heat duty are number of 8, 4.44308 and 180000MJ/h respectively in order to maximize recovery of acids and solvent. For the distillation column 2, optimum feed stages location, reflux ratio and re-boiler heat duty are number of 23, 10.5 and 3000MJ/h respectively in order to maximize purity of acrylic acid. For overall result, it was found that by optimizing the operating conditions of units, desired quality of products is improved and more materials is recovered.

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

Acrylic acid becomes more important in our daily life due to its wide applications such as its use in the manufacturing of plastic, coating, paper coating, polishes paint formulations, leather finishing, polymers, textile industries and adhesive. Hence, production of acrylic acid is increasing from year to year in order to fulfill the human needs. Due to this reason, amount of production of acrylic acid in the acrylic plant is also increasing. At the same time, acrylic plant must be able to maintain the same desired quality of acrylic acid by optimizing operating conditions in reactor and separation sections.

In the industry, the complicated problems of chemical plant are not always solved by human due to the human errors and time constraints (Bernards & Overney, 2004). There are many types of simulation programs that are used in industry which depends on the application, desired simulation products and the field of industry. Aspen plus is a powerful tool for Chemical Engineering in various fields including oil and gas production, refining, chemical processing, environmental studies, and

power generation (Bernards & Overney, 2004). Therefore, Aspen Plus simulator is chosen for this study.

In present work, the acrylic acid production plant is simulated and optimized by using Aspen Plus software. The plant has two major sections which consist of reactor and separation section. In the reactor section, propylene undergoes oxidation reactions to become acrylic and acetic acid. In the separation section, products undergo five separation units in order to obtain the desired products. These five main separation units consist of flash drum, absorption tower, liquid-liquid extractor, and two units of distillation columns. Separation efficiency of each separation unit depends on operation conditions which will directly affect the amount of loss of materials, operating cost, and the desired quality of the final products.

Optimization plays an important role in order to obtain the desired quality of acrylic and acetic acids. Before carrying out the optimization, steady state simulation of the acrylic acid plant must be first simulated. Therefore, reactor and separation sectors can be optimized in order to maximize the profits, reduce energy consumption, get higher processing rates, reduce maintenance cost, and have longer time between shutdowns. The optimization parameters consists of reflux ratio, feed stages location, temperature, pressure, re-boiler heat duty and flow rate of solvent that used in whole acrylic acid plant for optimization. Therefore, it is able to produce more amount of acrylic acid with desired quality in order to fulfill the demand in the market. Apart from that, it can provide a lot of insight before actual plant commissioning is done.

1.2 Problem Statement

Nowadays, the amount of acrylic acid production is become more from year to year due to its variety applications in order to fulfill human basic needs. Hence, due to this reason, the production of acrylic acid in acrylic plant must be increased also in order to meet the required demand. When the amount or capacity of production is increase in the acrylic plant, all the operating conditions of reactor and separation sections must be adjusted to another new optimum condition in order to maintain the desired purity products. Therefore, the acrylic acid plant has to precede optimization in order to overcome a large amount of acrylic acid production.

Moreover, vapor recovery system and liquid recovery system play an important role in recover or recycle back of the reactants and products such as propylene, acrylic acid, and acetic acid in order to prevent them being released into the environment, save raw material cost and increase more revenue. According to the Acrylic Acid MSDS (2005) and Acetic Acid MSDS (2005), acrylic acid and acetic acid are potentially hazardous material which will bring effect on living things' respiratory system, eyes, skin, or ingestion. Apart from that, loss of materials can cause the economic loss of that company and accidents incident may occurs because propylene is a flammable gas. Hence, optimization on this two recovery system can prevent the loss of hazardous materials to the environment, economic loss and improve safety in the acrylic acid plant.

1.3 Research Objectives

The objectives of this study are:

I. To simulate a production of acrylic acid process.

II. To optimize the operating conditions in reactor and separation sections of acrylic acid plant.

1.4 Research Questions

The research questions of this study are:

I. How to simulate a production of acrylic acid process?

II. How to optimize of operating conditions in reactor and separation sections of acrylic plant?

1.5 Scope of Study

The main objectives of this research are to optimize the reactor and separation sections in the production of acrylic acid process. In order to obtain the result, we have limited our research within a scope which consists of:

I. Simulation of acrylic acid plant by using Aspen Plus software.

II. Optimization parameter for plug flow reactor is only temperature.

III. Optimization parameters of the separation section are reflux ratio, feed tray location, pressure, temperature, molar flow rate of solvent and re-boiler duty only.

1.6 Expected Outcome

From this study, it is expected that by running the models and simulations on Aspen Plus software, each operating conditions and selection will be more understandable so that the optimized condition can be achieved for an acrylic acid plant. Besides that, all units such as plug flow reactor, flash drum, absorption unit, liquid-liquid extractor, two units of distillation columns in acrylic acid plant are expected to be optimized at the optimum conditions. Furthermore, an environmental friendly acrylic acid plant is expected to be achieved by reducing loss of hazardous materials to environment.

1.7 Significance of Study

The first significance is in the terms of publication. If this study were to be published, the findings can be read or researched again by others in order to simulate and optimize the acrylic plant again. The acetic acid, propylene and acrylic acid are hazardous materials which can harm all living things. However, this study is able to minimize the loss of hazardous materials to the environment so that the acrylic acid plant can become more environments friendly and have a higher safety aspect. Apart

from that, this study is carried out so as to get a better design of acrylic acid plant with all separation units under optimum conditions. Furthermore, by conducting this study, a higher quality of desired products which include acrylic acid and acetic acid by optimizing the separation units in acrylic acid plant can be obtained. Lastly, this study is also able to maximize the profits, reduced energy consumption, higher processing rates, reduced maintenance cost, and longer time between shutdowns.

CHAPTER 2

LITERATURE REVIEW

2.1 Products of Acrylic Acid Plant

2.1.1 Acrylic Acid

The main product of the acrylic plant is acrylic acid which is a clear, colorless liquid at ambient temperature and pressure (Cascieri and Clary, 1993). It can be described as a pungent, rancid, irritating, acrid and sweet (Verschueren, 1996). One of the applications of acrylic acid is used as a starting material in the production of acrylic esters and as a monomer for polyacrylic and polymethacrylic acid and salts (Genium, 1999). Besides that, it is also used as a co-monomer for polymers used as flocculants and for polymers used in molding powder, construction units, decorative emblems and insignias (Genium, 1999). Moreover, acrylic acid is used in the manufacturing of plastics, in polymer solutions for coatings, in paint formulations for leather finishing, in paper coatings, in polishes and adhesives and in general finishes and binders (Genium, 1999). According to the Acrylic Acid MSDS (2005), acrylic acid is very hazardous when in contact with skin (permeator), corrosive to skin and eye contact, skin contact may produce burn, and irritation of respiratory tract.

2.1.2 Acetic Acid

Another product of acrylic plant is acetic acid. It is by-product which produced during oxidation of propylene process. Acetic acid is an organic compound with the chemical formula CH_3COOH. It is a colorless liquid and has a distinctive sour taste and pungent smell. It is used in manufacturing of drugs, dyes, plastics, food additives and insecticides (Malvda, 2007). Acetic acid is one of the simplest and most widely used carboxylic acids having many chemical and industrial applications. Total worldwide production of acetic acid is about 6.5 million tons per year; out of which about 5 million tones are produced by methanol carbonylation process and by bacterial fermentation and the remaining 1.5 million tons by recycling (Production Report, 2005). According to the Acetic Acid MSDS (2005), it is very hazardous in case of skin contact (irritant), of eye contact (irritant), and of inhalation. Besides that, it is classified as a weak acid, but concentrated acetic acid is corrosive and attacks the skin.

2.1.3 Physical and Chemical Properties

The physical and chemical properties of acrylic acid and acetic acid are summarized in Table 2.1.

Table 2.1 Physical and Chemical Properties of Acrylic Acid and Acetic Acid (Ahmed, 2002)

Properties	Acrylic Acid	Acetic Acid
Molecular Weight	72.06 g/mol	60.05 g/mol
Physical State	Liquid	Liquid
Melting Point	12.3 ℃	16.66 ℃
Boiling Point	141 ℃	117.9 ℃
Specific Gravity (liquid)	1.05 (20 ℃)	1.049
Specific Gravity (gas)	2.5	2.07
Vapor Pressure	3.2mmHg (20 ℃)	15.7mbar
Solubility in Water	Miscible	Miscible
Solubility	Miscible in alcohol, benzene, chloroform, ether, acetone, DMSO	Miscible in diethyl ether, acetone, alcohol, glycerol, benzene
Pka	4.3	4.75
Henry's Law Constant	3.2×10^{-7}	9.3×10^{-2} (25 ℃)
Octanol Water Partition Coefficient (log K_{ow})	0.31 – 0.46	-
Organic Carbon Partition Coefficient (K_{oc})	2.21 L/kg	-
Flash Point	54 ℃	40 ℃
Explosive Limits	2.4% to 8.04%	19.9%
Auto ignition Temperature	390 – 446 ℃	400 ℃

2.2 Current Industrial Process

There are several chemical pathways to produce acrylic acid, and one of the most common ways is via the partial oxidation of propylene. The chemical reaction mechanism for producing acrylic acid involved two step processes in which propylene is first oxidized to acrolein and then further oxidized to acrylic acid. Each chemical reaction step usually takes place over a separate catalyst and at different operating conditions. The chemical reaction is in the equation (1) and (2).

$$C_3H_6 + O_2 \rightarrow C_3H_4O + H_2O \quad (1)$$

Acrolein

$$C_3H_6O + \frac{1}{2}O_2 \rightarrow C_3H_4O_2 \quad (2)$$

Acrylic acid

However, there are some several major side reactions which may occur due to the oxidation of reactants and products. The major side reactions are given below in equation (3), (4) and (5).

$$C_3H_4O + \frac{7}{2}O_2 \rightarrow 3CO_2 + 2H_2O \quad (3)$$

$$C_3H_4O + \frac{3}{2}O_2 \rightarrow C_2H_4O_2 + CO_2 \quad (4)$$

Acetic Acid

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O \quad (5)$$

Therefore, the reactors have to be operated at suitable conditions with catalyst so that can maximized the production of acrylic acid (Richard et al., 1998, pp. 716-727).

2.2.1 Reaction Kinetics and Reactor Configuration

The reactions of oxidation propylene are all irreversible because the equilibrium lies far to the right hand side (Richard et al., 1998, p. 716). The reaction kinetics with the catalyst used in the acrylic plant process is given in the Table 2.2

which follows the chemical equation (6), (7), and (8). The partial pressure of reactants and products are in kPa.

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O \quad (6)$$

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow C_2H_4O_2 + CO_2 + H_2O \quad (7)$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O \quad (8)$$

where $-r_i = k_{0,i}\exp\left(-\frac{E_i}{RT}\right)P_{propylene}P_{oxygen}$

Table 2.2 Activation Energies and Pre-exponential Terms for Reaction Number of 6 to 8 (Richard et al., 1998)

i	E_i (kcal/kmol)	$k_{o,i}$ (kmol/m^3reator//h/(kPa)^2
6	15,000	1.59 x 10^5
7	20,000	8.83 x 10^5
8	25,000	1.81 x 10^8

According to the Richard et al. (1998), the kinetic presented in the Table 2.2 are valid in temperature range of 250 ℃ until 330 ℃ only. When the temperature is above 330 ℃, the catalyst starts to coke up due to the carbon deposits on the surface of catalyst. However, when the temperature is below 250 ℃, the rate of reaction will drop rapidly. Therefore, the optimum range of temperature for the reactor should be in the range of 250 ℃ until 330 ℃.

2.2.2 Process Flow Diagram

According to the Richard et al. (1998), the process flow diagram of oxidation of propylene are given in the Figure 2.1 and Figure 2.2 which is used to model the acrylic acid plant in Aspen Plus flow sheet. However, waste treatment unit in the process flow diagram is not considered in the constructing the flow sheet.

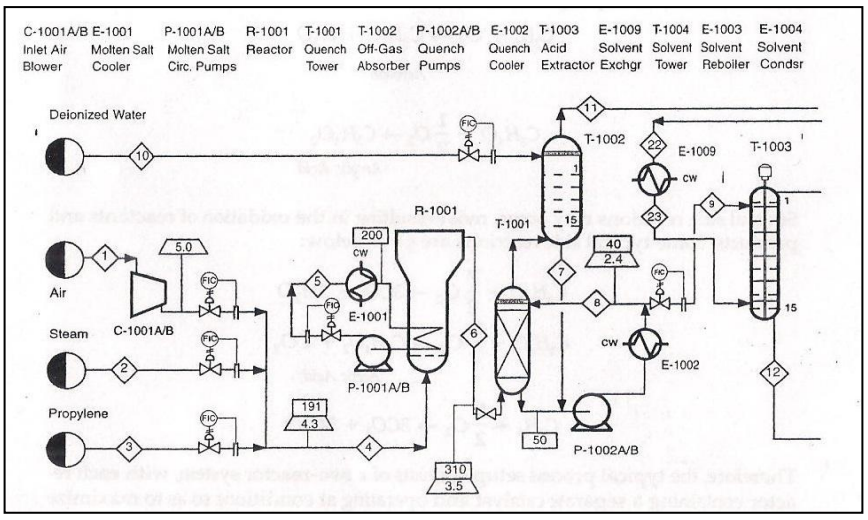


Figure 2.1 Preliminary Process Flow Diagram (PFD) for the Production of Acrylic Acid from Propylene (Richard et al., 1998)

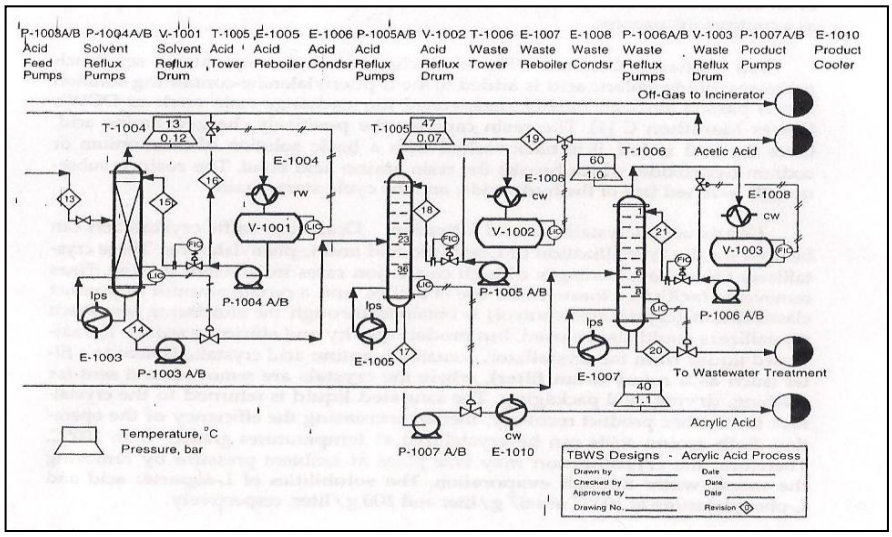


Figure 2.1 (Continued)

As another sources of process flow diagram, according to the Jamillah et al. (2000), their final process flow sheet of acrylic acid plant is shown in Figure 2.3. It is used as another reference of simulation model in Aspen Plus flow sheet. Apart from that, based on Richard (1998), the basic amount of production of acrylic acid is 50,000 metric tons per year of 99.9 mole % of acrylic acid product and the number of operating hours should be taken as 8000/yr. Besides that, the flow summary of each stream and preliminary equipment summary in acrylic acid plant are shown in the Table 2.3 and 2.4 (Richard et al,. 1998).

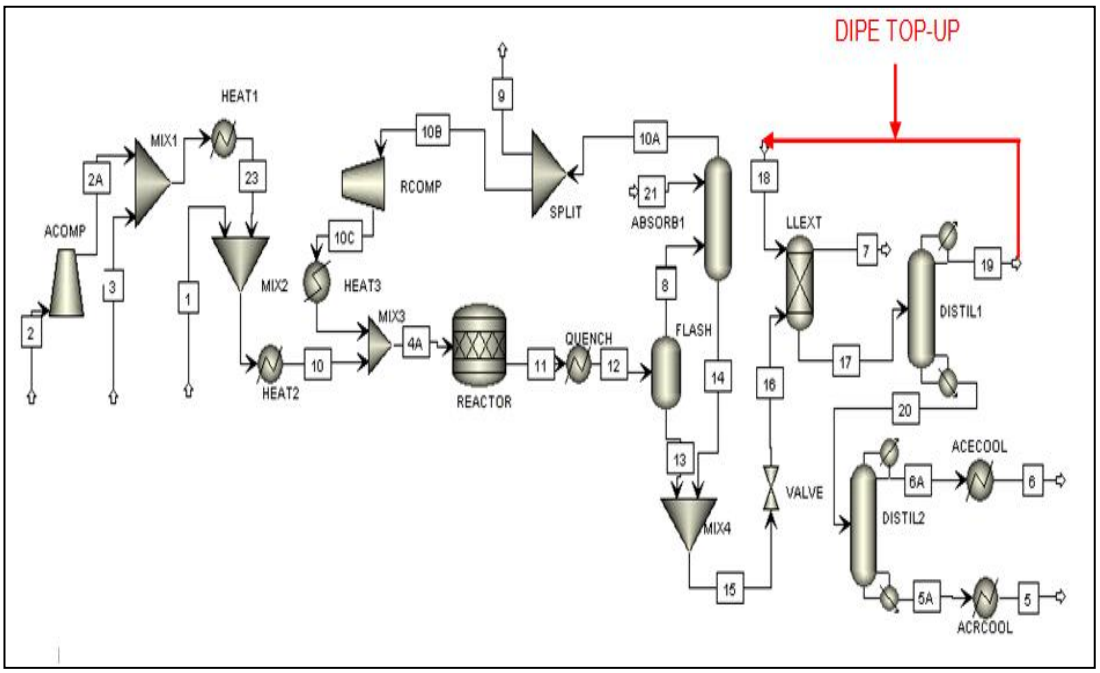


Figure 2.2 Process Flow sheet of Acrylic Acid Plant (Jamillah et al., 2000)

Table 2.3 Flow Summary Table for Acrylic Acid Process (Richard et al., 1998)

Stream Number	1	2	3	4	5	6	7	8
Temperature (◦C)	25	159	25	191	250	310	63	40
Pressure (bar)	1.0	6.0	11.5	4.3	3.0	3.5	1.4	2.4
Vapor fraction	1.0	1.0	1.0	1.0	0.0	1.0	0.00	0.00
Mass flow (tone/h)	39.05	17.88	5.34	62.27	1075.0	62.27	3.08	1895
Mole flow (kmol/h)	1362.9	992.3	127.0	2482.2	0.00	2444.0	148.5	85200.0
Component mole flow (kmol/h)								
Propylene	0.00	0.00	127.0	127.0	0.00	14.7	0.00	0.00
Nitrogen	1056.7	0.00	0.00	1056.7	0.00	1056.7	0.00	0.00
Oxygen	280.9	0.00	0.00	280.9	0.00	51.9	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	60.5	0.00	0.00
Water	25.3	992.3	0.00	1017.6	0.00	1165.9	140.9	78870
Acetic Acid	0.00	0.00	0.00	0.00	0.00	6.54	0.65	415
Acrylic Acid	0.00	0.00	0.00	0.00	0.00	87.79	6.99	5915
Solvent(DIPE)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 2.3 (Continued)

Stream Number	9	10	11	12	13	14	15	16
Temperature (◦C)	40	25	48	40	40	90	13	13
Pressure (bar)	2.4	5.0	1.0	2.4	2.4	0.19	0.12	3.0
Vapor fraction	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
Mass flow (tone/h)	27.46	2.54	37.35	20.87	143.0	6.63	155.3	136.4
Mole flow (kmol/h)	1249.6	141.0	1335.4	1156.9	1591.2	93.19	1705.7	1498.0
Component mole flow (kmol/h)								
Propylene	0.00	0.00	14.7	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	1056.7	0.00	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	51.9	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	60.5	0.00	0.00	0.00	0.00	0.00
Water	1156.7	141.0	150.2	1156.6	198.8	0.30	226.0	198.5
Acetic Acid	6.08	0.00	0.46	0.03	6.08	6.08	0.00	0.00
Acrylic Acid	86.81	0.00	0.98	0.00	86.81	86.81	0.00	0.00
Solvent(DIPE)	0.00	0.00	0.00	0.30	1299.5	0.00	1479.7	1299.5

Table 2.3 (Continued)

Stream Number	17	18	19	20	21	22	23
Temperature (◦C)	89	47	47	102	60	13	40
Pressure (bar)	0.16	0.07	1.1	1.1	1.0	3.0	2.8
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass flow (tone/h)	6.26	5.28	0.37	20.84	37.37	136.4	136.4
Mole flow (kmol/h)	86.85	90.49	6.34	1156.43	470.2	1498.5	1498.5
Component mole flow (kmol/h)							
Propylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water	0.00	4.28	0.30	1156.4	126.8	198.7	198.7
Acetic Acid	0.05	86.07	6.03	0.03	0.00	0.00	0.00
Acrylic Acid	86.80	0.14	0.01	0.00	0.00	0.00	0.00
Solvent(DIPE)	0.0	0.00	0.00	0.00	343.4	1299.8	1299.8

Table 2.4 Preliminary Equipment Summary for Acrylic Acid Process (Richard et al., 1998)

Equipments	T-1001	T-1002	T-1003	T-1004	T-1005	T-1006
MOC	Stainless Steel	Stainless Steel	Stainless Steel	Stainless Steel	Carbon Steel	Stainless Steel
Diameter (m)	5.3	3.5	2.2	7.5	2.4	2.3
Height/ length (m)	12	11	9.5	34	25	7.0
Orientation	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical
Internals	10m of High-efficiency Packing Polyethylene	15 Sieve Trays + Demister Stainless Steel	15 Perforated Plates + Mixer Stainless Steel	31m of High-efficiency Structured Packing Stainless Steel	36 Sieve Plates Stainless Steel	8 Sieve Plates Stainless Steel
Pressure (barg)	1.4	1.0	1.4	-1.0	-1.0	0

2.2.3 Process Description

Firstly, the raw materials which consist of air, steam, and propylene are mixed together before feed into reactor. The chemical reactions taken place on a single catalyst to convert the feed mixture into acrylic acid and by-products. After the reactants reacted in the reactor, the outlet stream of the reactor is at 310℃ and is in gaseous state. The outlet stream of reactor contains water and acidic compounds (acetic acid and acrylic acid) with dipoles, and non-ideal behavior would be exhibited (Jamillah et al., 2007, p.7). In order to avoid further oxidation reactions, the product stream is cooled down rapidly by quenching with a cool recycle stream of dilute aqueous acrylic acid in the flash drum (T-301).

The function of flash drum is used to separate out vapor and condensed liquid. The outlet stream of flash drum is fed to two general separation system which are vapor recovery system and liquid recovery system. The outlet vapor is fed to the vapor recovery system and the outlet condensed liquid is fed to the liquid recovery system.

In the acrylic acid plant, the separator that used as a vapor recovery system is the absorption unit. When the two containing phases are gas and a liquid, this operation is called as absorption (Christie, 2003, p. 625). Since some of the acetic acid and acrylic acid leaving from the flash drum are in gas phase, hence they are recovered back by using deionized water (liquid phase) as a solvent. This is because to acrylic acid and acetic acid has an infinite solubility in deionized water (Perry and Green, 1997). Due to the corrosive materials of acrylic acid, water and acetic acid,

design material for the absorption columns is by using stainless steel materials. According to the King (1980), sieve trays are chosen because have similar efficiency to bubble-trays and less 30% until 50% cost.

For the liquid recovery system, there are three units involved which are liquid-liquid extractor, and two distillation columns. Firstly, liquid-liquid extractor, which is also called as acid extractor, has liquid inlet stream which contains three components. They are acrylic acid, acetic acid and water and it used diisopropyl ether (DIPE) as a solvent. As a description of liquid-liquid extraction, when the two contacting phases are liquids, where a solute or solutes are removed from one liquid phase to another liquid phase, the process is called liquid-liquid extraction (Christie, 2003, p. 626). Hence, liquid-liquid extractor is suitable to be used as a separation unit among acrylic acid, acetic acid and water. Besides that, diisopropyl ether is used as a solvent due it has high solubility for acrylic acid and acetic acid but low solubility for water (Richard et al., 1998, p. 717). Therefore, water is easily separated out from the mixture and then undergo wastewater treatment unit before release to the environment. However, acetic acid, acrylic acid and diisopropyl ether is fed into the first distillation column for further separation. Apart from diisopropyl ether, there are many other possible solvents that can be used to separate the acrylic acid such as ethyl acrylate, ethyl acetate, xylene, diisobutyl ketone, and methyl isobutyl ketone.

After that, the outlet stream of liquid-liquid extractor is fed into distillation column 1 in order to separate out the diisopropyl ether as the top product. It is recycled back to the liquid-liquid extractor and used as solvent again. However, the mixture of acrylic acid and acetic acid (bottom products) is fed to the second

distillation column in order to obtain the desired products. The distillation column is chosen as the separation unit because volatile vapor phase and liquid phase that vaporizes are involved (Christie, 2003, p. 626). During the second distillation column, due to the low boiling point of acetic acid but high boiling point of acrylic acid, acetic acid becomes the vapor phase and acrylic acid becomes the liquid phase. Therefore, acetic acid is the top product but acrylic acid is the bottom product.

2.3 Simulation

A simulation is the operation of a model of a system. In the simulation, the model can be reconfigured and experimented with too expensive or impractical to do in the system it represents. On the other words, simulation is a tool to evaluate the performance of a system, existing or proposed, under different configurations of interest and over long periods of real time (Andradottir et al., 1997). The simulator that used in this study is Aspen Plus which is a component of Aspen Engineering Suite™ (AES).

2.3.1 Aspen Plus Simulator

Aspen Plus is a powerful tool for Chemical Engineering because it runs a process simulation model by providing a comprehensive system of online prompts, hypertext help, and expert system guidance at every step (Aspen Plus: Getting Started Building and Running a Process Model, 2010). The process of simulation is

applied in chemical engineering which consists of many chemical components such as mixed, separated, heated, cooled, and converted by unit operations. Besides that, Aspen Plus can solve the critical engineering and operating problems that arise throughout the lifecycle of a chemical process (Luyben, 2010). For example, design a new plant or processes, troubleshooting a process unit, and optimizing operations such as acrylic acid plant. There are some functions for using Aspen Plus Process Simulation:

I. Predict the behavior of process by using basic engineering relationships, such as mass and energy balances, or chemical equilibrium.
II. Simulate actual plant behavior when given reliable thermodynamics data, realistic operating conditions, and rigorous equipment models.
III. Perform model analysis such as sensitivity analysis, case study, or constraints.
IV. Perform optimization runs for equipments or processes.
V. Design better plants and increase profitability in existing plants.

2.3.2 Aspen Property Models

One of the elements in the Aspen Plus Simulation is the base and property methods which is used to characterize the fluid behavior. The chosen base and property method is able to accurately model with particular stream conditions or characteristics. Due to the polar components in the acrylic acid plant which consists of water, acetic acid and acrylic acid, the system exhibited a high degree of non-ideal behavior. Besides that, according to Jamillah et al. (2007), the acetic acid-acrylic

acid-water mixture is azeotropic in nature which is another reason for the non-ideal behavior. There are some recommended property methods for every chemical reaction processes which is given in the Table 2.5. Therefore, the chosen base method is NRTL-RK and the property models employed are UNIF-LL, UNIFAC and UNIF-DMD in the liquid-liquid extractor, absorber, and distillation columns respectively (Jamillah et al., 2007, p. 9).

Table 2.5 Recommended Property Methods for Chemicals (Aspen Plus ®: Aspen Plus User Guide, 2000)

Application	Recommended Property Methods
Azeotropic separation	WILSON, NRTL,UNIQUAC
Carboxylic acids	WILS-HOC, NRTL-HOC, UNIQ-HOC
Phenol plant	WILSON, NRTL, UNIQUAC
Liquid phase reactions	WILSON, NRTL, UNIQUAC
Ammonia plant	PENG-ROB,RK-SOAVE
Fluorochemicals	WILS-HF
Inorganic chemicals	ELECNRTL
Hydrofluoric acid	ENRTL-HF

According to Jamillah (2007), UNIFAC is used as a predictive model for the mixture's behavior in the event that the binary parameters for the system are not included in the Aspen databanks. Hence, it is very accurate in modeling the VLE data. Therefore, it is suitable to be applied for the absorption tower since the system involves the dissolution of the acidic gases in the water. Besides that, UNIF-LL is based on the previously described UNIFAC property method and is able to accurately model LLE data (Jamillah, 2007). This property is suitable in the liquid-liquid extraction column in order to get accurate modeling of the interaction between organic solvent and acidic solution. Furthermore, UNIF-DMD is also based on the UNIFAC method which contains more temperature dependent terms of the group-group interaction parameters (Jamillah, 2007). Hence, it is suitable for distillation

column and flash drum because both involve VLE and LLE interactions and separation is based on relative volatility.

2.3.3 Equipments Selection

2.3.3.1 Reactor

Aspen Plus provides seven models of reactors for chemical reactor simulation which are RStoic, RYield, REquil, RGibbs, RCSTR, RPlug, and RBatch. Each reactor models have their own purpose which is shown in the Table 2.6.

Table 2.6 Purpose of Reactor Models in Aspen Plus Software

Model	Purposes
RStoic	Conversion reactor with known stoichiometry
RYield	Yield reactor with known product yields
REquil	Two-phase chemical equilibrium reactor (stoichiometric)
RGibbs	Multiphase chemical equilibrium reactor (non-stoichiometric)
RCSTR	Continuous stirred tank reactor with known kinetics
RPlug	Plug flow reactor with known kinetics
RBatch	Batch or semi-batch reactor with known kinetics

The heats of reaction are not required for reactor model because Aspen Plus calculates heats of reaction by using heat of formation. RStoic model is selected to be used as a reactor because the chemical stoichiometry of this oxidation of propylene in equation 6, 7, and 8 are known. Besides that, this model can specify the extent of each chemical reaction or conversion. Apart from that, RStoic can handle reactions that occur independently in a series of reactors and perform product selectivity and heat of reaction calculations (Aspen Plus ®: Aspen Plus User Guide, 2000).

2.3.3.2 Separators

There are five different type of model of separation in Aspen Plus which are Flash2, Flash3, Decanter, Sep and Sep2. The purpose of each separator is shown in Table 2.7.

Table 2.7 Purpose of Separator Models in Aspen Plus Software (Aspen Plus ®: Aspen Plus User Guide, 2000)

Model	Purposes
Flash2	Perform rigorous 2 (vapor-liquid) phase equilibrium calculations and produces one vapor stream, one liquid outlet stream, and optional water decant stream.
Flash3	Perform rigorous 3 phase vapor-liquid-liquid equilibrium calculation and to produce one vapor outlet stream and two liquid outlet streams.
Decanter	Decanter models required sufficient residence time for separation of two liquid phases but without a vapor phase.
Sep	Sep combines inlet streams and separates the resulting stream into two or more streams by according to splits specify for each components.
Sep2	Sep2 combines inlet streams and separate the resulting stream into two outlet streams. It is similar to Sep but offers a wider variety of specifications which are purity and recovery.

When the outlet stream comes out from the reactor, the products are at 310 ℃ and gaseous phase. According to the Figure 2.1, the outlet of reactor is fed to the flash drum unit and the outlet vapor and liquid phases of flash drum are fed to the vapor recovery system and liquid recovery system respectively. Hence, Flash2 is selected as the flash drum unit because it produced one vapor outlet stream and one liquid outlet stream. Besides that, this unit can specify percentage of the liquid phase to be entrained in the vapor stream.

2.3.3.3 Columns

Columns in Aspen Plus software have nine types of models which are DSTWU, Distl, SCFrac, RadFrac, MultiFrac, PetroFrac, RateFrac, BetchFrac, and Extract. The purpose of each models of column is shown in Table 2.8.

Table 2.8 Purpose of Column Models in Aspen Plus Software (Aspen Plus ®: Aspen Plus User Guide, 2000)

Model	Purposes
DSTWU	It designs calculation for a single-feed, two-product distillation column with a partial or total condenser. It can estimate reflux ratio by given the number of theoretical stages, number of theoretical stages by given the reflux ratio, optimum feed stage location, and condenser and re-boiler duties.
Distl	It is a shortcut multi-component distillation rating model and separate an inlet stream into two products. It required specifying number of theoretical stages, reflux ratio and overhead product rate.
SCFrac	It models petroleum refining towers and performs shortcut distillation calculation for columns with a single feed, one optional stripping steam stream, and any number of products.
RadFrac	It is a rigorous model for simulation all types of multistage vapor-liquid fractionation operations. It can simulate absorption, re-boiled absorption, stripping, re-boiled stripping, and extractive and azeotropic distillation. It is suitable for three phases' systems, narrow boiling or wide boiling systems, and systems exhibiting strong liquid phase non-ideality.
MultiFrac	It is a rigorous model for simulating multistage fractionation unit. It can models a complex configuration consisting of any number of column but each with any number of stages, any number of connections between columns or within column and arbitrary flow splitting or mixing of connecting streams.
PetroFac	It is a rigorous model designed for simulating complex vapor-liquid fractionation operations in the petroleum refining industry. Typical operations include pre-flash tower, FCC main fractionators, delayed coke main fractionators, and vacuum lube fractionators.
RateFrac	It is a rate-based model for non-equilibrium separation. It simulates single and interlinked columns involving vapor-liquid fractionation operations such as absorption, distillation and stripping. It can be used for systems with both a vapor and a liquid phase, nonreactive system, reactive system, and electrolyte systems.

Table 2.8 (Continued)

BatchFrac	It is a rigorous model for simulating multistage batch distillation columns. It can handle a wide variety of batch distillation problems which include narrow-boiling, wide-boiling highly non-ideal, three phase and reactive systems.
Extract	It is a rigorous model for simulating liquid-liquid extractors. It can have multiple feeds, heaters/coolers, and side-streams. In order to calculate distribution coefficients, this model should specify which are activity coefficient models, or equation of state capable of representing two liquid phases.

As mentioned before, the vapor outlet stream from the flash drum is fed to the vapor recovery system. The equipment that is selected is the absorption unit in order to recover back the acrylic acid and acetic acid before being released to the environment. In the Aspen Plus, there are two kinds of columns that can be used to simulate absorption unit which are RadFrac and RateFrac. However, ABSORBER in the RateFrac is chosen because it involving vapor-liquid fractionation operations and nonreactive system. RadFrac is not suitable because the system did not have three phases, narrow or wide boiling system and any strong liquid phase non-ideality are not present.

There are three separation units involved in the liquid recovery system which are the liquid-liquid extractor, and two distillation columns. For the liquid-liquid extractor, Extract is chosen because only one extractor is being used in Aspen Plus. For the other two distillation columns, Distl is chosen because it separated an inlet stream into two products (Luyben, 2006). Besides that, it just only required to specify number of theoretical stages, reflux ration and overhead product rate.

2.4 Optimization Method in Aspen Plus

In the Aspen Plus simulator, it contains the function of optimization in the model analysis tools in order to analyze the simulation process. The functions of model analysis tools include sensitivity analysis, optimization, constraint, data fit, and case study. For the optimization purpose, sensitivity analysis and optimization are selected to be use for optimization on acrylic acid plant. As a definition of optimization, it is the engineers work to improve the initial design of equipment and strive to enhance the operation of that equipment (Thomas and David, 2001, p. 4). Optimization can bring a lot of benefits and advantages for any plants because it can realize the largest production, greatest profit, minimum operating cost, and least energy usage. Furthermore, optimization can also lead to reduced maintenance costs, less equipment wear, and better staff utilization.

There are essentially two type of optimization. The first is termed as topological optimization and deals with the topology or arrangement of process equipment (Richard et al., 1998, p. 510). The second type is known as parametric optimization and it deals with the operating variables, such as temperature, pressure or reflux ratio for a given piece of equipment or process (Richard et al., 1998, p. 510). In this study, parametric optimization method is chosen to progress the optimization process on the acrylic acid plant.

2.4.1 Sensitivity Analysis

Sensitivity Analysis is a tool for determining how a process reacts by varying the key operating and design variables (Aspen Plus ®: Aspen Plus User Guide, 2000). The changes made to a flow sheet input quantity in a sensitivity block do not affect the simulation and so, it runs independently of the base-case simulation. The results of Sensitivity Analysis are reported in a table on the Sensitivity Results Summary sheet. The first n columns of the table list the values of the variables that are varied, where n is the number of varied flow sheet variables entered on the Sensitivity Input Vary sheet. The remaining columns in the table contained the values of variables that were tabulated in the Tabulated sheet.

The function of sensitivity analysis is to vary one or more flow sheet variables and study the effect of that variation on other flow sheet variables. Hence, it is a valuable tool for performing the "what if" study for these variables but the flow sheet variables that are varied must be the inputs to the flow sheet. Besides that, it is used to verify if the solution to a design specification lies within the range of the manipulated variable. Apart from that, another main function is used to perform a simple process optimization for the process. Moreover, it is used to generate tables and plot of simulation results as functions of feed stream, block input, or other input variables in order to provide additional information to base-case results, but have no effect on the base-case simulation.

2.4.2 Optimization

The function of optimization in the model analysis tools is used to maximize or minimize a user-specified objective function by manipulating decision variables. Objective function is a mathematical function that provides the best values of the decision variables which will reach a minimum or a maximum (Richard et al., 1998, p. 510). Hence, it is goodness or measurement for the optimization. For optimization, when the optimum measurement is a profit, it should be maximize, but when optimum measurement is a cost, it should be minimize. The objective function can be any valid Fortan expression involving one or more flow sheet quantities.

Before using the function of optimization, constraints must be imposed in the model analysis tools. Constraints are limitations on the values of decision variables. As stated before, the definition of design variables is those independent variables where the engineer has some control (Richard et al., 1998, p. 509). Anyway, constraint is divided into two categories which are equality constraint and inequality constraint (Richard et al., 1998, p. 510). The equality constraints within an optimization are similar to design specifications and it can be any function of flow sheet variables computed using Fortran expressions or in-line Fortran statements.

According to the Aspen Plus Guide (2000), there are some recommended procedure for creating an optimization problem which are:

i. Start with a simulation because it is easier to detect flow sheet errors. Next, determine the reasonable specifications, a reasonable range of decision variables and get a good estimate for the tear streams.

ii. Perform sensitivity analysis before optimization in order to find appropriate decision variables and their ranges.

iii. Evaluate the solution using sensitivity analysis in order to find out if the optimum is broad or narrow.

2.4.3 Parameters for Optimization of Separation Units of Acrylic Acid Plant

In optimizing a chemical process, the key decision variables have to be identified correctly and early in the optimization procedure. This is because it reduced the computational effort and time taken for optimizing the process (Soo et al, 1998). If the decision variables cannot be identified correctly, it will consume a lot of time to carry out an optimization and computational effort. The choice of decision variables is crucial to the efficiency of the optimization process. There are some important variables that must always be considered for most chemical process which include the operating conditions for reactor, single-pass conversion in the reactor, recovery of unused reactants, purge ratios for recycle streams, purity of products, reflux ratio and components recovery in columns, and finally, the operating pressure of separators (Richard et al., 1998, pp. 540-541). Therefore, optimized parameters that are used for acrylic acid plant are identified in the Table 2.9.

Table 2.9 Parameters for Optimization of Separation Units

Separation Units	Parameters for Optimization
Absorption tower	Number of stages and solvent flowrate
Liquid-liquid extractor	Number of stages and solvent flowrate
Distillation column 1	Reflux ratio, feed trays location, and reboiler duty
Distillation column 2	Reflux ratio, feed trays location, and reboiler duty

CHAPTER 3

METHODOLOGY

3.1 Introduction

The study is carried out by using Aspen Plus software to simulate and optimize the acrylic acid plant. The simulation is used to evaluate the performance of the acrylic acid plant and solved the critical engineering and operating problems. For the optimization, it is obtained the optimum conditions for each reactor and separation sections in the acrylic acid plant. Generally, the methodology is divided into three parts which are Phase I: Steady state simulation; Phase II: Sensitivity analysis; Phase III: Optimization. The first phase is described how to simulate a steady state of acrylic acid plant in the flow sheet. The second phase is described how to analysis the design variables for all the models by using Sensitivity Analysis. Lastly, the third phase is described how to use optimization to maximize or minimize a user-specified objective by manipulating decision variables.

Before start to optimize the acrylic acid plant, firstly, simulation of acrylic acid plant is started so that a reasonable range of decision variable is determined. Secondly, sensitivity analysis has performed before the optimization because it used

to find appropriate decision variables and their ranges. After two previous steps are done, the optimization is carried out and relationship among four phases is shown in Figure 3.1.

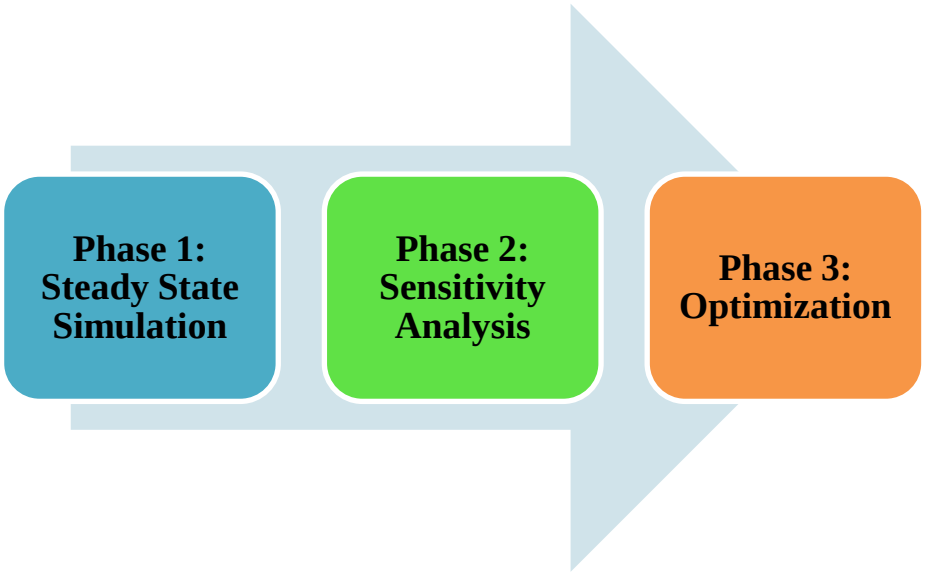


Figure 3.1 General Procedures for Optimization

3.2 Phase I: Steady State Simulation

There are six steps to simulate a steady state of acrylic acid plant which are construct flow sheet, specify components, specify property method, specify stream's condition, specify block condition and run the simulation. A flow chart of steady state simulation is shown on Figure 3.2.

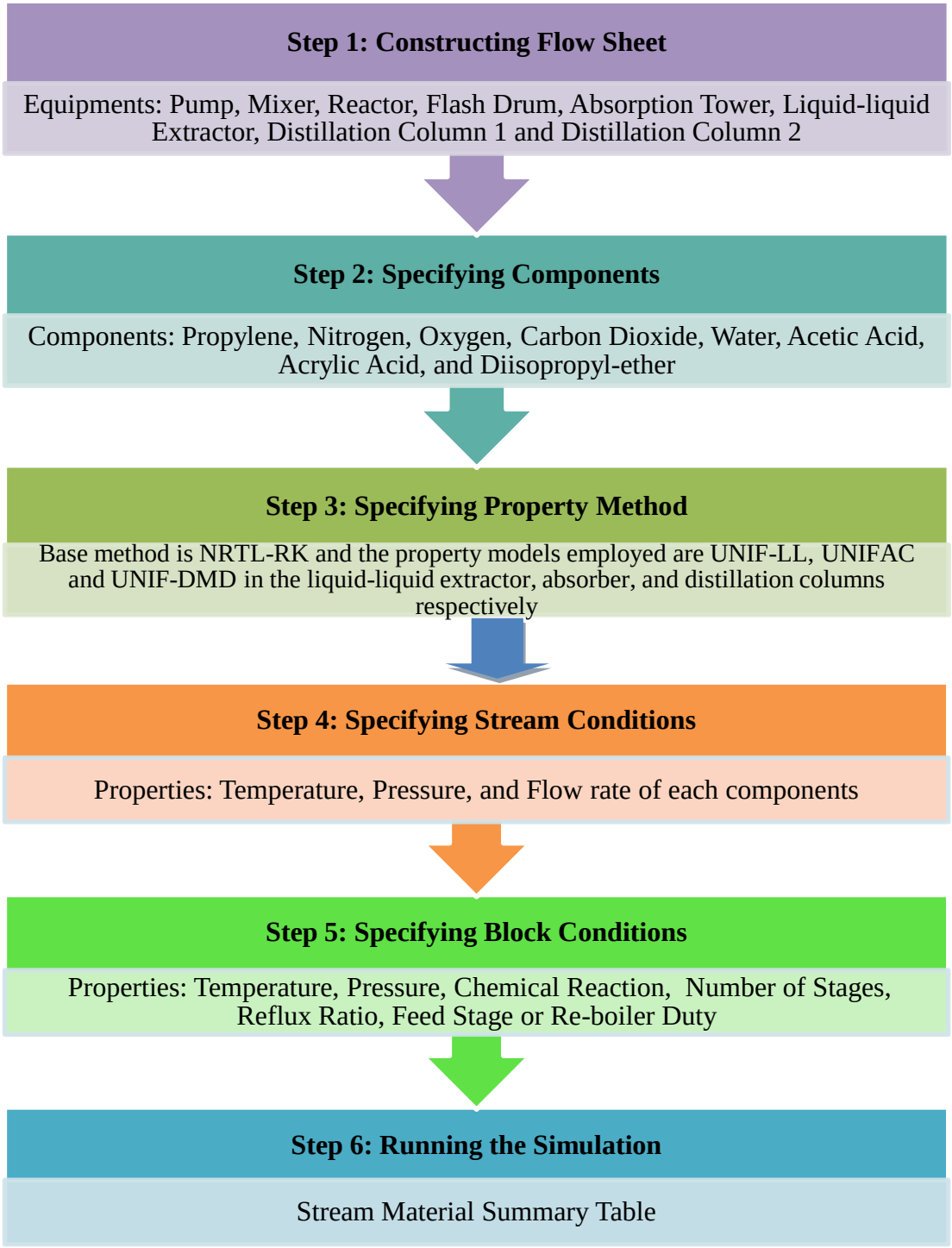


Figure 3.2 Brief Flow Chart on Steady State Simulation

3.2.1 Step 1: Constructing Flow Sheet of Acrylic Acid Plant

The Aspen Plus flow sheet is a section to displays the process flow sheet for the simulation. It includes group of blocks, pumps, heaters, or flow streams in order to simplify viewing if the simulation. According to the Figure 2.1, 2.2, and 2.3, a flow sheet of acrylic acid plant in aspen plus is simplified as Figure 3.3. The name for equipments is listed in the Table 3.1.

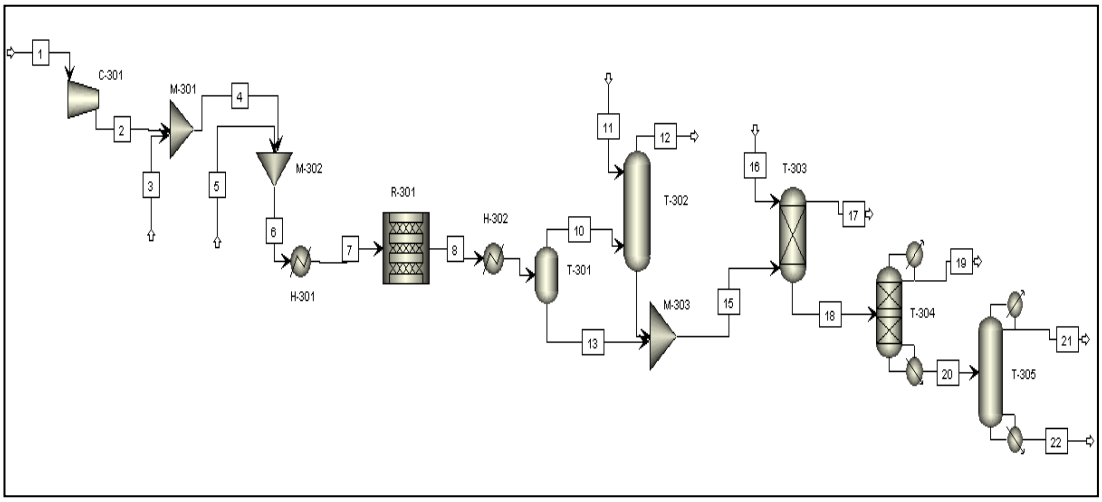


Figure 3.3 Flow Sheet for the production of Acrylic Acid Plant in Aspen Plus

Table 3.1 Name of Equipments

Symbols	Name of Equipments
C-301	Inlet Gas Blower
H-301	Heat Exchanger 1
H-302	Heat Exchanger 2
M-301	Mixer 1
M-302	Mixer 2
M-303	Mixer 3
R-301	Plug Flow Reactor
T-301	Flash Drum
T-302	Absorption Tower
T-303	Liquid-liquid Extractor
T-304	Distillation Column 1
T-305	Distillation Column 2

3.2.2 Step 2: Specifying Components

In the acrylic acid plant, the chemical components involved in the reactor and separation sections are propylene, nitrogen, oxygen, carbon dioxide, water, acetic acid, acrylic acid, and diisopropyl-ether. All of these components are found in the Aspen Plus Databank. In order to select chemical components, firstly, from the Data menu, Components button is clicked. Find dialog box is used to enter the search criteria for these components such as component name or formula, component class, molecular weight, boiling point, or CAS number. Figure 3.4 shows that finding propylene component in the Find Dialog Box.

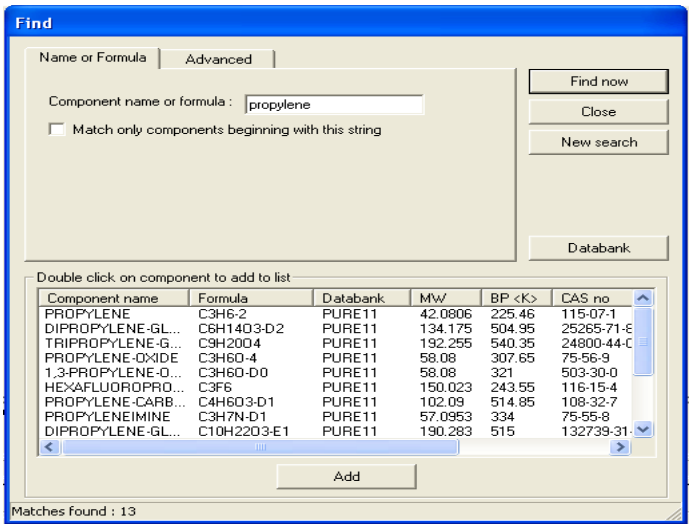


Figure 3.4 Find Dialog Box

After the components searched by Find Dialog Box, then correct chemical components are selected from the list and Add button is clicked in order to add it to the components list. After all of these chemical components are selected, the components list is seen like Figure 3.5.

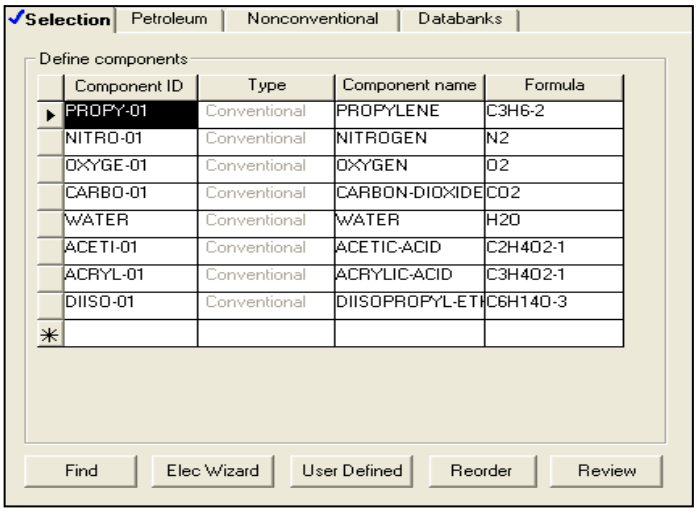


Figure 3.5 Component List

3.2.3 Step 3: Specifying Property Method

In Aspen Plus, the global property method for all property calculations, but some of the equipments used different property methods which are absorption unit, liuid-liquid extractor, distillation column 1 and distillation column 2. As mentioned previously, the chosen base method for whole simulation is NRTL-RK. In order to specify the global property method, the Properties from Data menu is clicked and then the property method is specified in the Property Method list. Once the property method is selected, the base method is automatically selected as same method. Figure 3.6 shows that the selection of property method in the Global sheet.

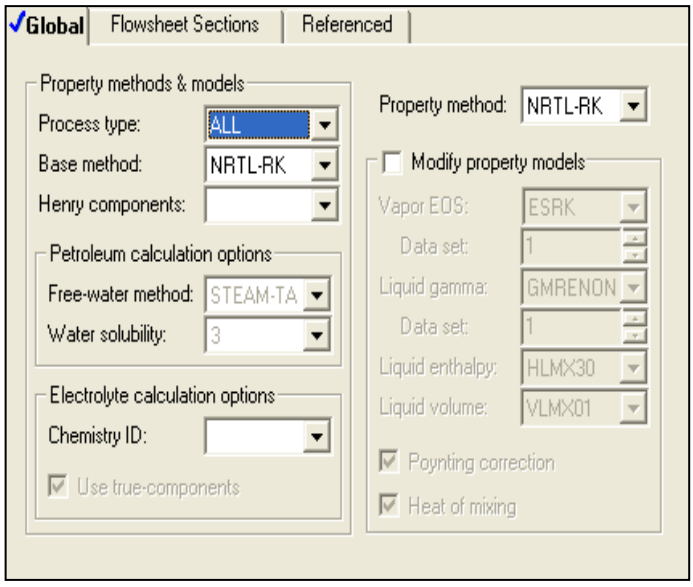


Figure 3.6 Global Sheet in Properties

As mention early, the property method employed in the liquid-liquid extractor, absorber, and distillation columns are not same with the base method and they are UNIF-LL, UNIFAC and UNIF-DMD respectively. In order to specify property method for the certain equipment, firstly, the Block from the Data Menu is clicked and the related units are selected. Then, the Block Option is clicked and related property method is selected in the Property Method. Figure 3.7 shows that the Properties sheet of liquid-liquid extractor.

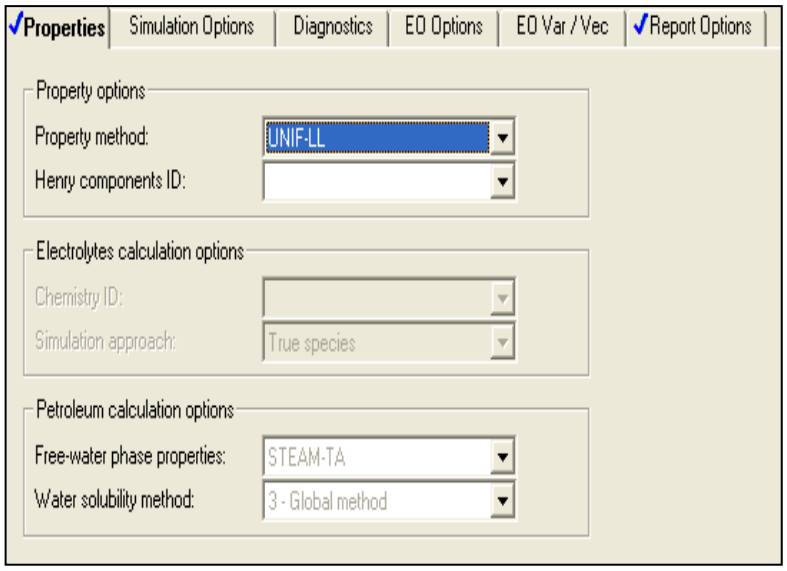


Figure 3.7 Properties Sheet of Liquid-liquid Extractor (T-303)

3.2.4 Step 4: Specifying Stream Conditions

For all material process, feed streams must be specified flow rate, composition and thermodynamic condition. In order to enter the specification for a stream, firstly, the Stream from the Data Menu is clicked. In the Streams Object Manager, the stream is selected and Edit is clicked. On the Specification sheet as shown in Figure 3.8, the thermodynamic condition of the streams are specified which include temperature, pressure and vapor fraction. Next, the stream composition is specified by using flow rate or flow fractions for each component. Table 3.2 shows that the streams conditions required to specify before running the simulation. All the stream number sequence is followed to the flow sheet in Figure 3.1.

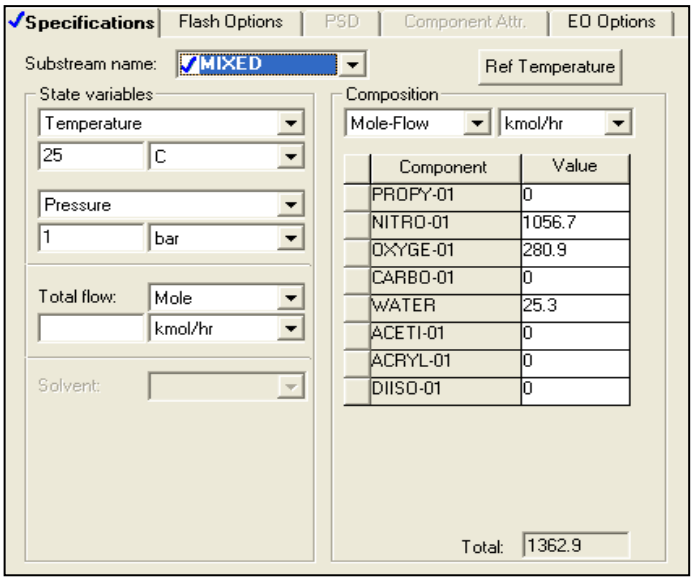


Figure 3.8 Specification Sheet of Stream 1

Table 3.2 Stream Condition of Stream 1, 3, 5, 11, and 16

Stream Number	1	3	5	11	16
Temperature (◦C)	25	159	25	25	40
Pressure (bar)	1.0	6.0	11.5	5.0	2.8
Vapor fraction	1.0	1.0	1.0	0.0	0.0
Component mole flow (kmol/h)					
Propylene	0.00	0.00	127.0	0.00	0.00
Nitrogen	1056.7	0.00	0.00	0.00	0.00
Oxygen	280.9	0.00	0.00	0.00	0.00
Carbon Dioxide	0.00	0.00	0.00	0.00	0.00
Water	25.3	992.3	0.00	141.0	198.7
Acetic Acid	0.00	0.00	0.00	0.00	0.00
Acrylic Acid	0.00	0.00	0.00	0.00	0.00
Solvent(DIPE)	0.00	0.00	0.00	0.00	1299.8

3.2.5 Step 5: Specify Block Conditions

The details block conditions must be specified according to the references before run the simulation. In the flow sheet of acrylic acid plant, there are totally twelve equipments which include reactor, flash drum, liquid-liquid extractor, two

distillation column and their conditions is accordingly to the Table 2.4. However, some of equipments such as compressor, mixer, and heat exchanger are depend on the outlet stream conditions required.

3.2.5.1 Compressor

There are only one compressor unit in the flow sheet and it is used to increase the pressure of air inlet stream before fed to the reactor. In the Specification Sheet, type of positive displacement compressor model is selected and 5 bar of discharge pressure is specified. Figure 3.9 shows that how to specify the specifications sheet of the compressor.

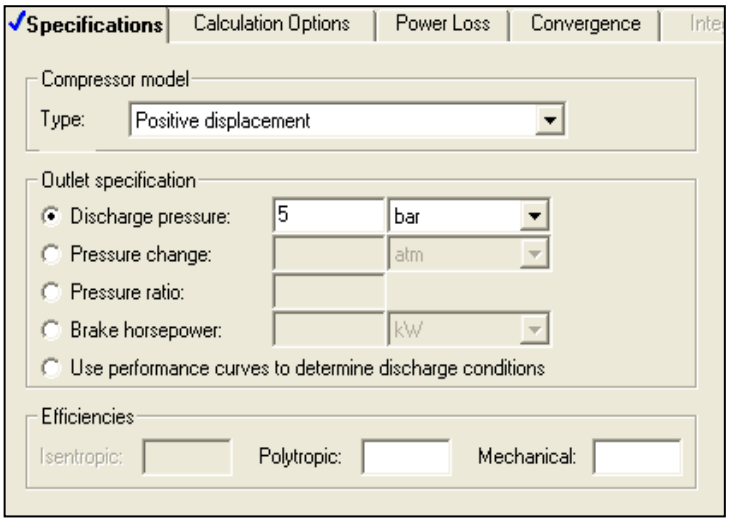


Figure 3.9 Specification Sheet of Compressor (C-301)

3.2.5.2 Mixer

In the flow sheet, there are three units of mixers which used to combines inlet material streams into one outlet stream. All their specifications of the mixer are based on the outlet streams conditions required. Figure 3.10 shows that how to specify the Flash Option sheet of Mixer-303 (M-303).

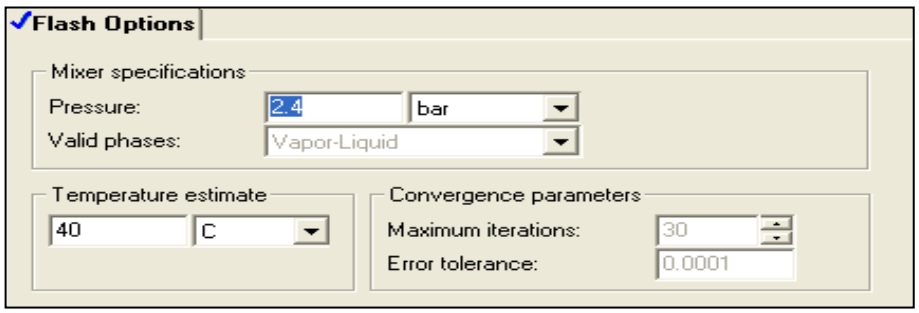


Figure 3.10 Flash Option Sheet of Mixer (M-303)

3.2.5.3 Heat Exchanger

There are two units of heat exchangers in the flow sheet which used to change the temperature and pressure among inlet and outlet streams. The specifications of heat exchanger are depends on outlet streams conditions. Valid phase for both heat exchangers is vapor-liquid only. Figure 3.11 shows that how to specify the specification sheet of Heat Exchanger-302 (H-302).

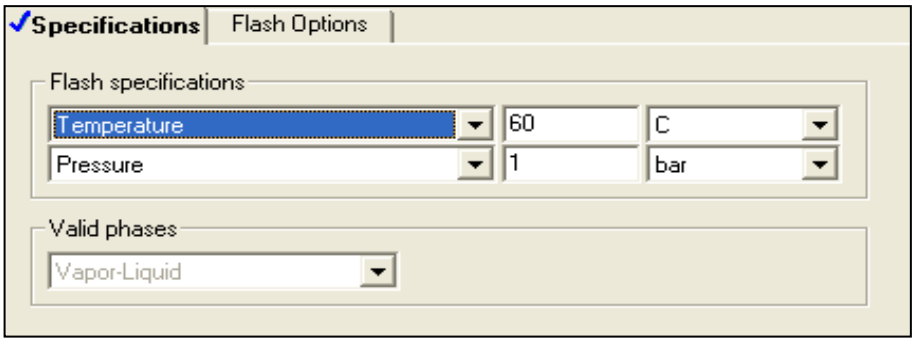


Figure 3.11 Specification Sheet of Heat Exchanger (H-302)

3.2.5.4 Reactor

RStoi in Reactors is used as a model of reactor in acrylic acid plant. According to the Richard et al (1998), the reactor is carried out in 310 ℃ and 3bar and the chemical reaction is oxidation of propylene which followed to the equation 6, 7, and 8. Figure 3.12 and 3.13 show that how to specify the Specification Sheet and Reactions Sheet respectively in reactor.

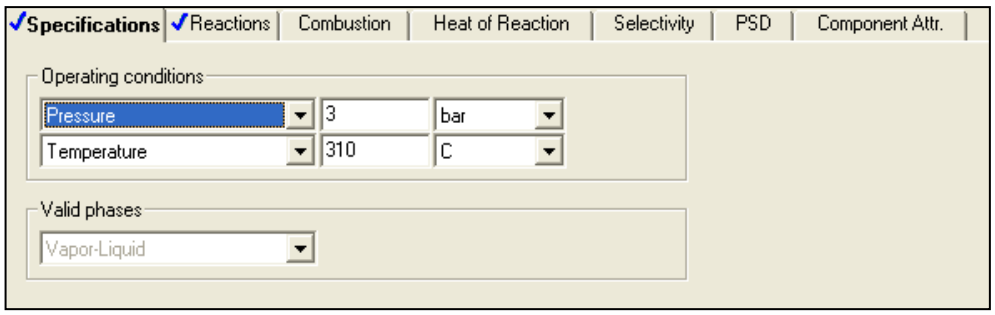


Figure 3.12 Specification Sheet of Reactor (R-301)

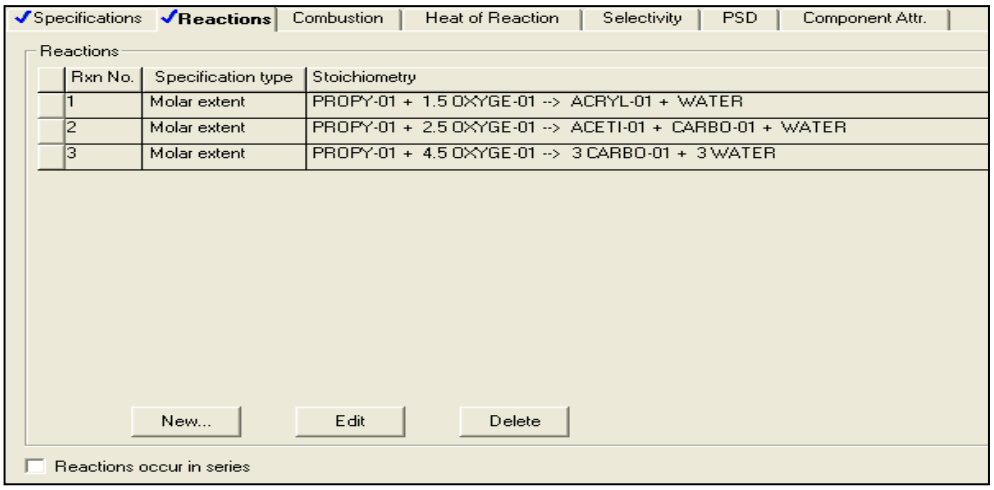


Figure 3.13 Reactions Sheet of Reactor (R-301)

3.2.5.5 Flash Drum

The outlet stream or product stream of reactor is then fed into flash drum at 40 ℃ and 2.4bar. The Flash2 in Separators is selected to be the flash drum unit. The valid phase of vapor-liquid is selected for the flash drum because outlet consists of vapor and liquid phases. Figure 3.14 show that how to specify the Specification Sheet of flash drum unit.

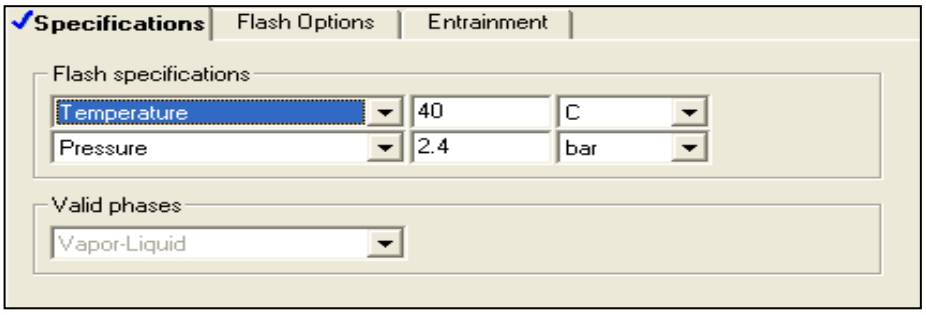


Figure 3.14 Specification Sheet of Flash Drum (T-301)

3.2.5.6 Absorption Unit

The outlet vapor stream from flash drum is fed to the absorption unit in order to recovery the acrylic acid and acetic acid. The ABSORBER in the RateFrac is selected to be the absorption unit. According to the Richard et al (1998), it has fifteen number of segment but do not have any condenser and re-boiler. Figure 3.15 shows that how to specify the Configuration Sheet of absorption column. Besides that, tray type of absorber is sieve trays and column diameter is 3.5 meter. The Specification sheet and Diameter sheet are shown in Figure 3.16 and 3.17 respectively. Lastly, Figure 3.18 shows that how to specify the inlet outlet of material stream in Materials Streams Sheet.

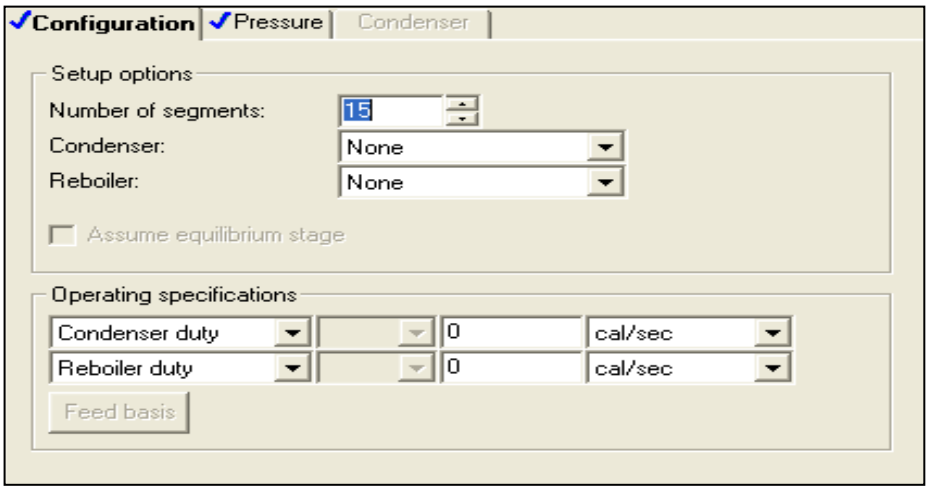


Figure 3.15 Configuration Sheet of Absorption Column (T-302)

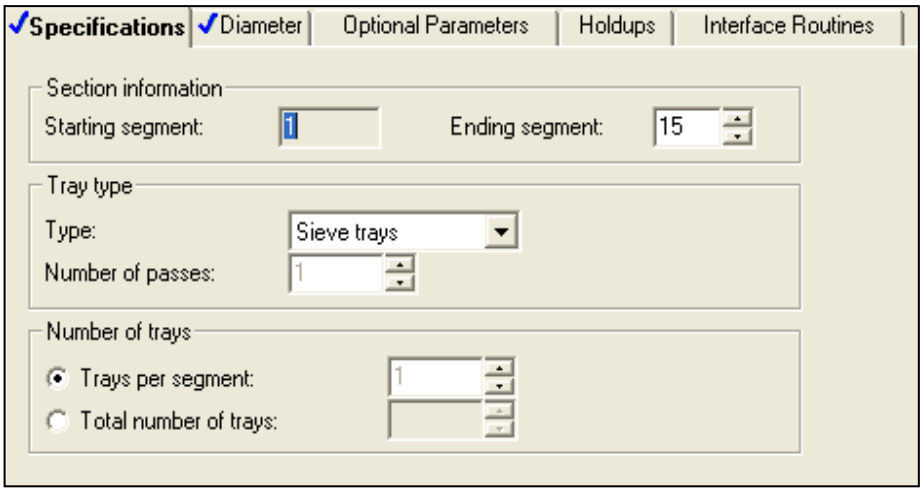


Figure 3.16 Specification Sheet of Tray in Absorption Column (T-302)

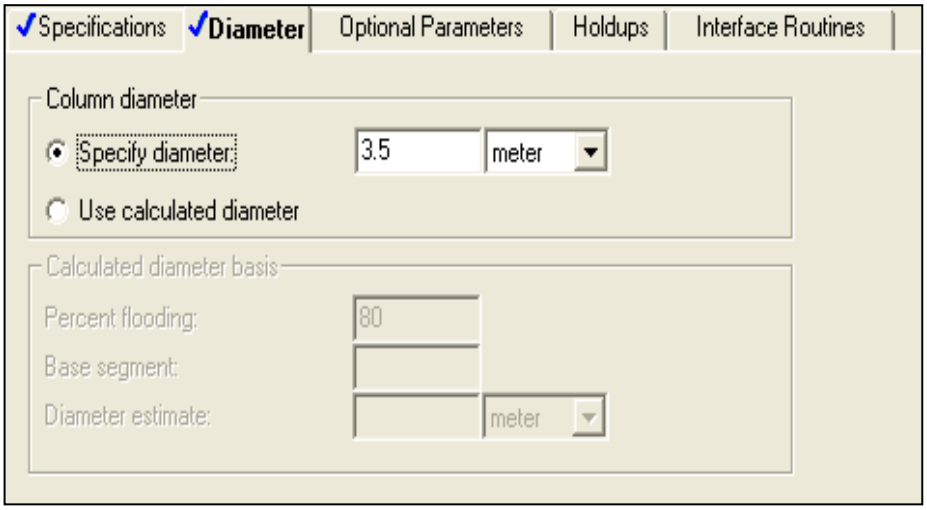


Figure 3.17 Diameter Sheet of Absorption Column (T-302)

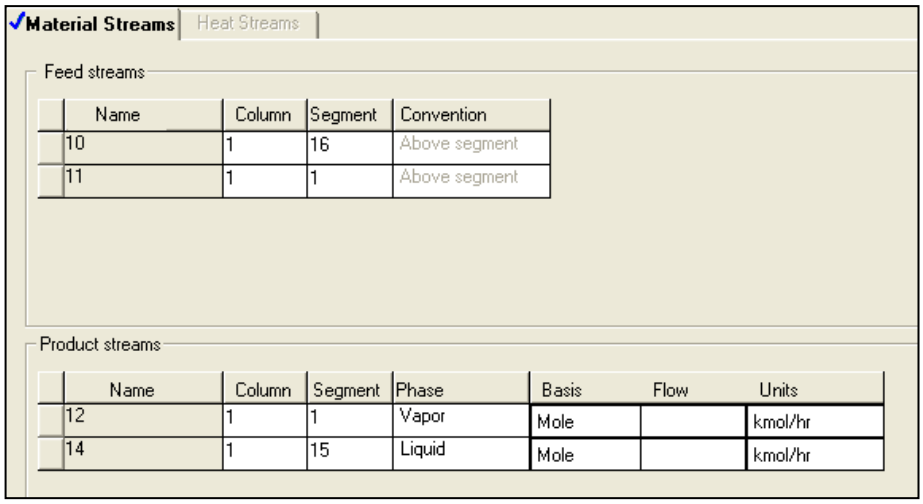


Figure 3.18 Material Streams Sheet of Absorption Column (T-302)

3.2.5.7 Liquid-liquid Extractor

The outlet streams of flash drum and absorption unit are combined together by mixer and then fed into liquid-liquid extractor in order to remove water by using diisopropyl-ether as a solvent. The model Icon 1 in the Extract is selected to be the liquid-liquid extractor. According to the Richard et al (1998), it contains fifteen number of stage in adiabatic thermal condition and operated in 1.4 barg. Figure 3.19 and Figure 3.22 shows that how to specify number of stage and pressure profile in the Specifications and Pressure sheets respectively. Moreover, key components required to specify in first and second liquid phases because it will influenced the composition of components in the product streams and Figure 3.20 shows how to specify the key components in liquid-liquid extractor. Next, location of feed, product streams, and liquid phases are specified accordingly to Figure 3.21.

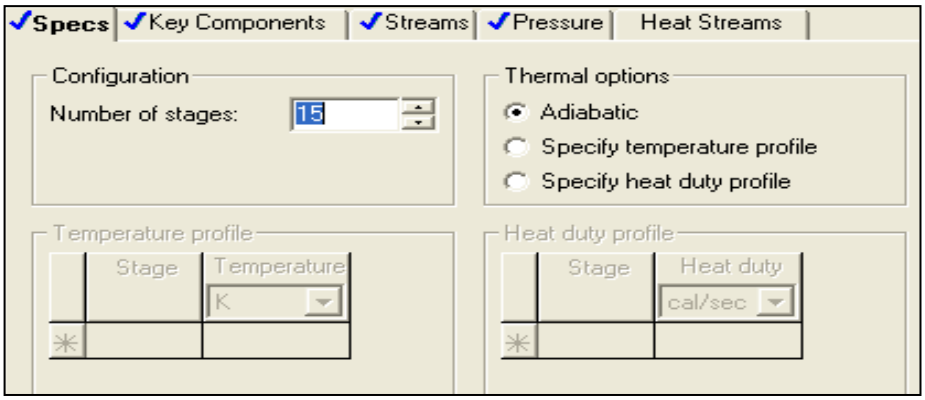


Figure 3.19 Specification Sheet of Liquid-liquid Extractor (T-303)

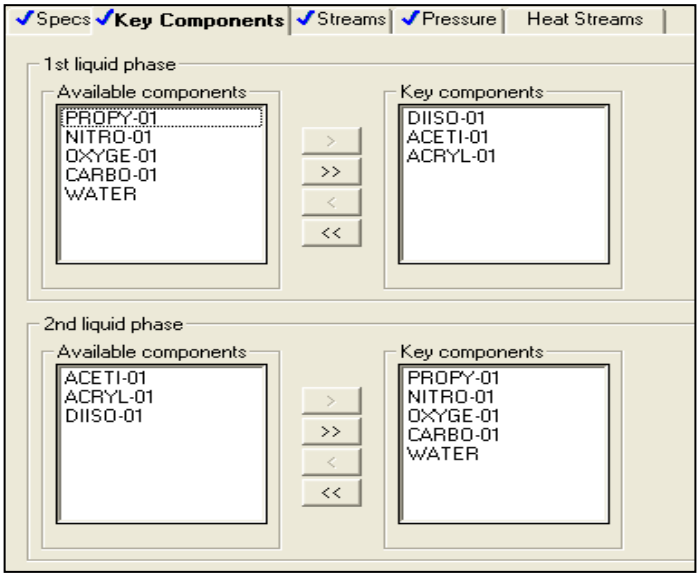


Figure 3.20 Key Components Sheet of Liquid-liquid Extractor (T-303)

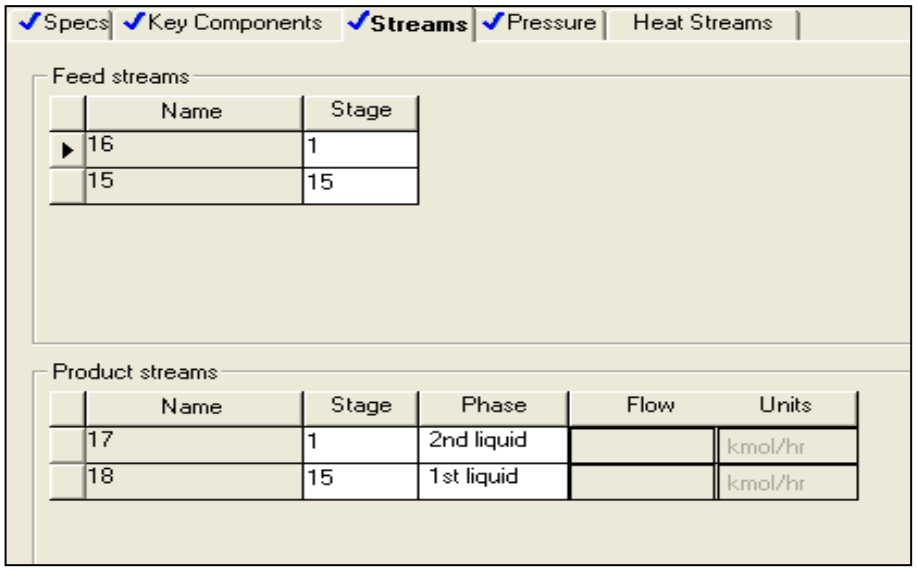


Figure 3.21 Streams Sheet of Liquid-liquid Extractor (T-303)

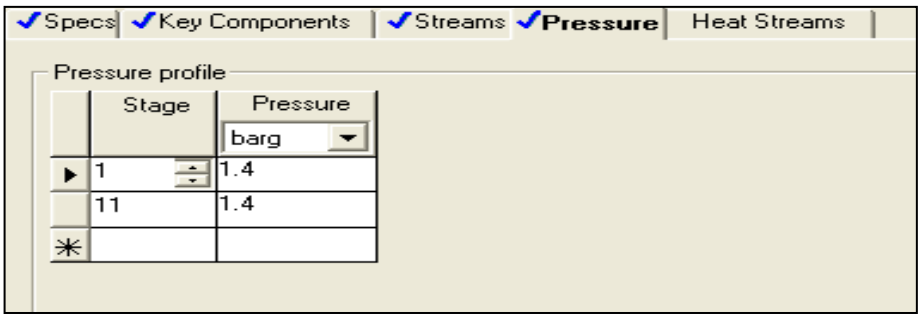


Figure 3.22 Pressure Sheet of Liquid-liquid Extractor (T-303)

3.2.5.8 Distillation Column 1

After the liquid-liquid extractor remove the excess water, one of the outlet stream is fed into distillation column 1 in order to remove and recycle back the diisopropyl-ether to the liquid-liquid extractor. The Icon2 in Distl is selected to be distillation column 1. In the column, the top product is diisopropyl-ether and bottom

product is acrylic acid and acetic acid. According to Jamillah et al. (2007), the distillation column 1 has fifteen numbers of stages, one total condenser and one re-boiler. Figure 3.23 shows that how to specify the Configuration Sheet of distillation column 1. Besides that, the feed stream in on stage number four and it operated at 0.1bar (Richard et al., 1998). The Stream Sheet and Pressure Sheet are shown in Figure 3.24 and Figure 3.25 respectively.

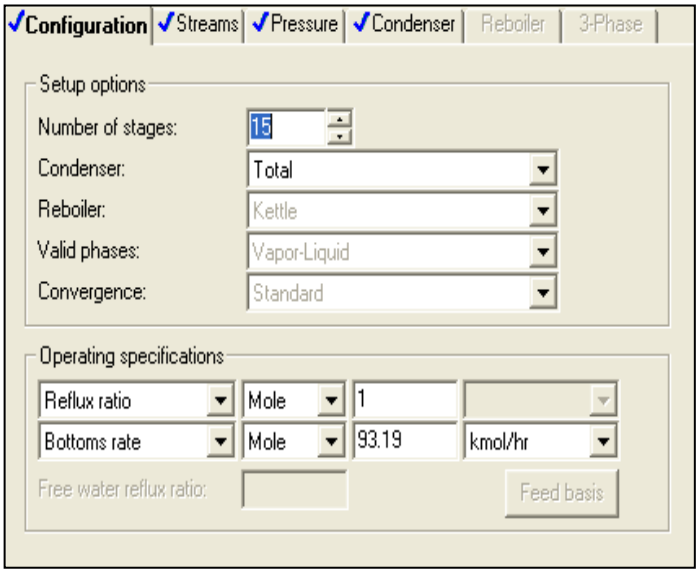


Figure 3.23 Configuration Sheet of Packed Distillation Column (T-304)

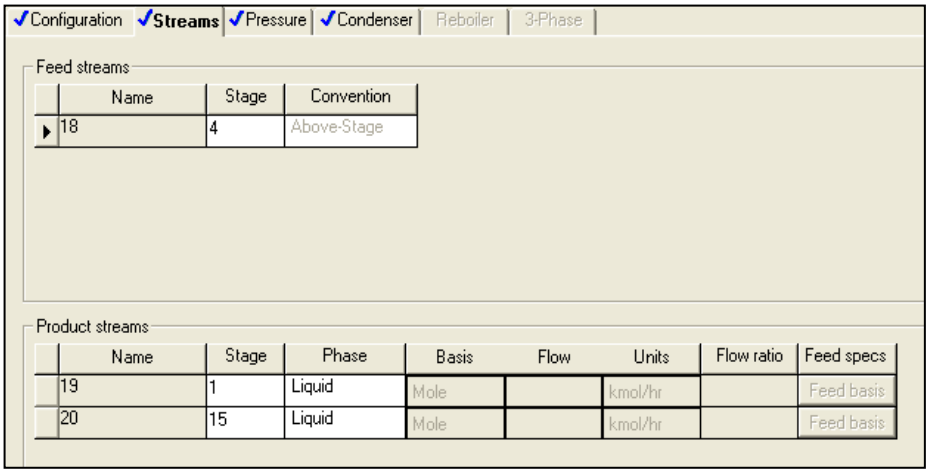


Figure 3.24 Streams Sheet of Packed Distillation Column (T-304)

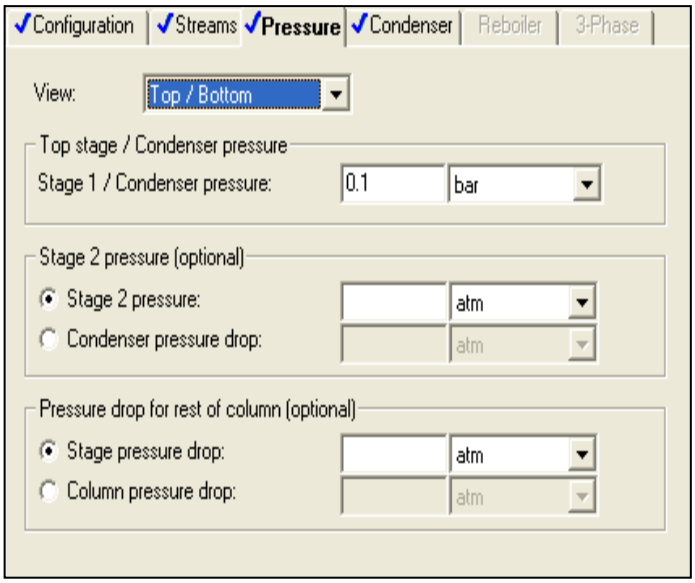


Figure 3.25 Pressure Sheet of Packed Distillation Column (T-304)

3.2.5.9 Distillation Column 2

Finally, the bottom product of packed distillation column is fed into second distillation column in order to obtain the desired products which are acrylic acid and acetic acid. The Icon1 in Distl is selected to be distillation column 2. According to Richard et al. (1998), the distillation column 2 has thirty-six numbers of stages, one total condenser and one re-boiler. Figure 3.26 show how to specify the Configuration Sheet of distillation column 2. Furthermore, the feed stream in on stage number twenty-three and it operate at -1.0barg. Figure 3.27 and 3.28 shows how to specify feed and product stream and pressure in the Stream Sheet and Pressure Sheet respectively.

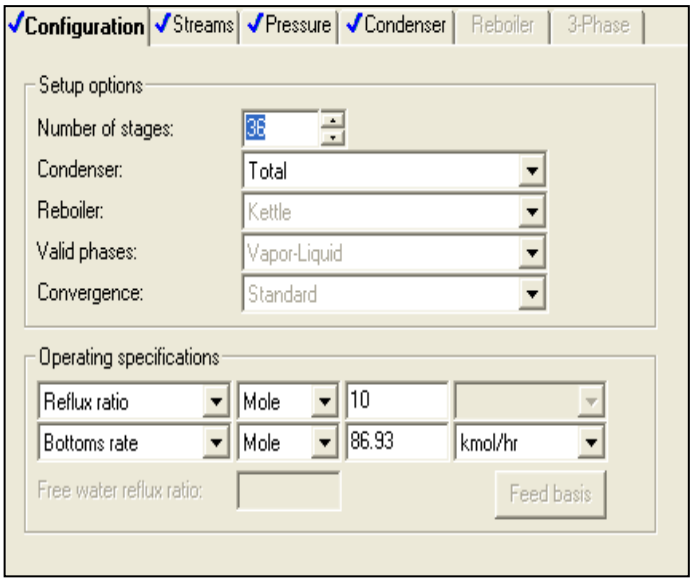


Figure 3.26 Configuration Sheet of Distillation Column (T-305)

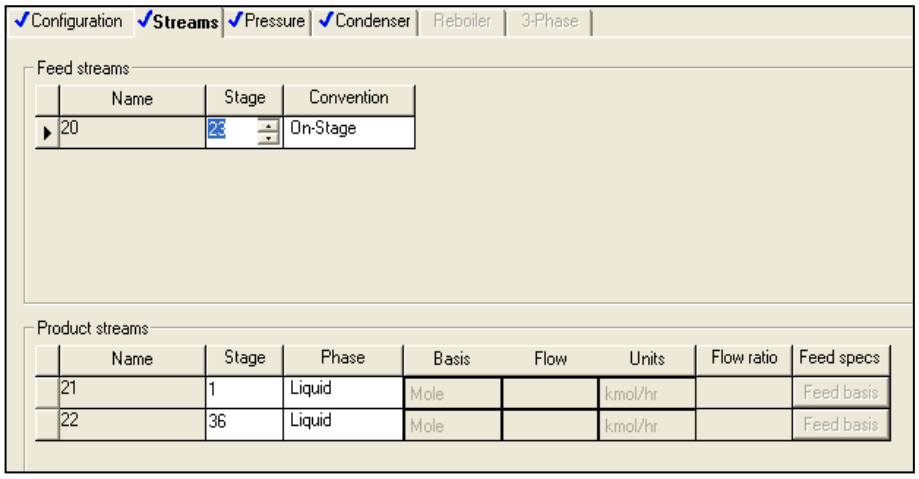


Figure 3.27 Streams Sheet of Distillation Column (T-305)

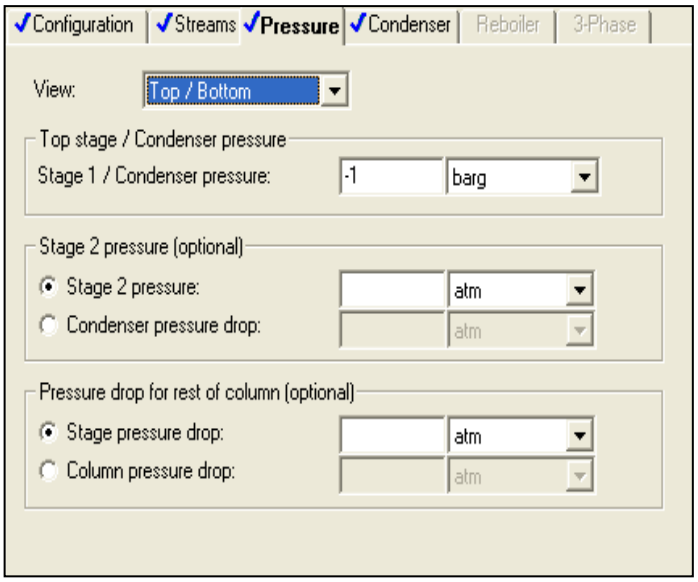


Figure 3.28 Pressure Sheet of Distillation Column (T-305)

3.2.6 Step 6: Running the Simulation

After all the previous steps are done, next step is run the simulation. Simulation is controlled by using the commands on the Run menu, the Simulation Run toolbar, or Control Panel. In order to run the simulation, from the Run menu, Run button is clicked.

3.3 Sensitivity Analysis

As mentioned previously, the optimization is involved two sections which are reactor and separation sections. Reactor section included optimized on plug flow reactor and separation section included flash drum, adsorption unit, liquid-liquid extractor, two distillation columns. Sensitivity analysis in Aspen Plus is used for

determining parameters of design variables and to perform simple process optimization. A brief flow chart of Sensitivity Analysis is shown in Figure 3.29.

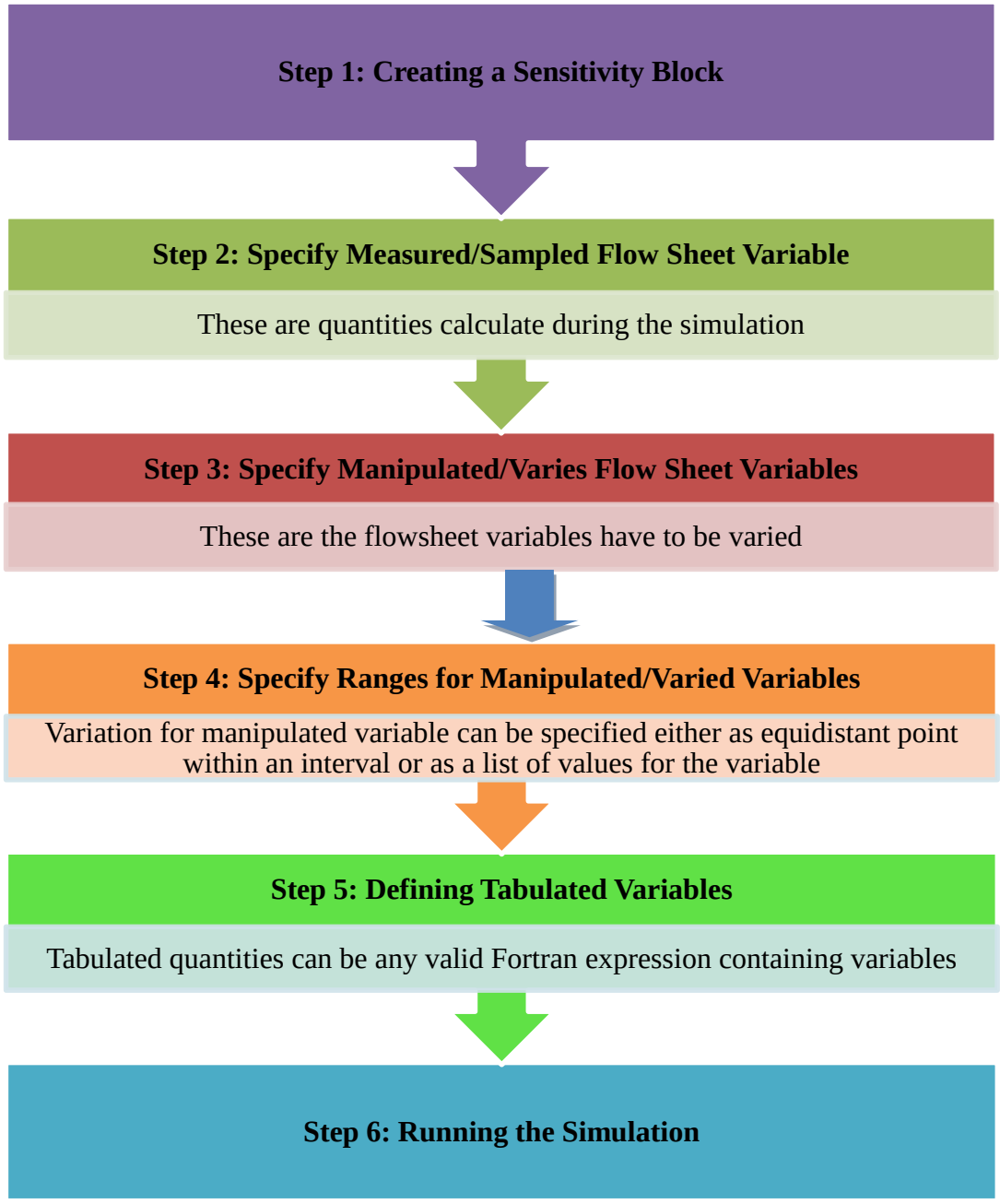


Figure 3.29 Brief Flow Chart on Sensitivity Analysis

3.3.1 Step 1: Creating Sensitivity Block

In order to create a sensitivity block, firstly, from the Data Menu, Model Analysis Tools is clicked and then Sensitivity. On the Sensitivity Object Manager as shown in Figure 3.30, New button is clicked. In the Create New ID dialog box as shown in Figure 3.31, an ID is entered, and then OK button is clicked.

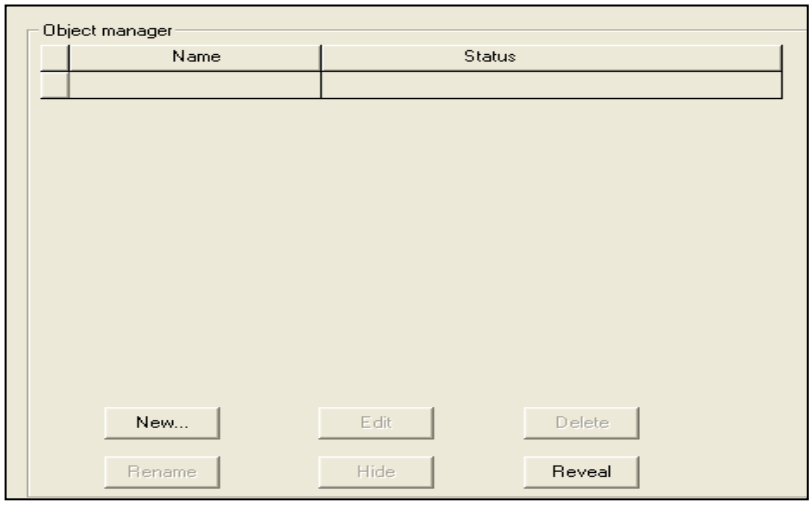


Figure 3.30 Sensitivity Object Manager

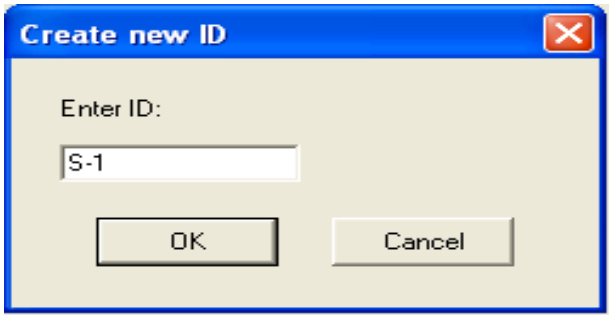


Figure 3.31 Create New ID Dialog Box

3.3.2 Step 2: Specify Measured/Sampled Flow Sheet Variables

For each sensitivity block, flow sheet variables must be identify and assigned them variable name. These variables can either tabulate or use in Fortran expression to compute tabulated results. The Define Sheet as shown in Figure 3.32 is used to identify a flow sheet variable and assign the variable name. When completing a Define Sheet, the variables is specified on the Variable Definition dialog box.

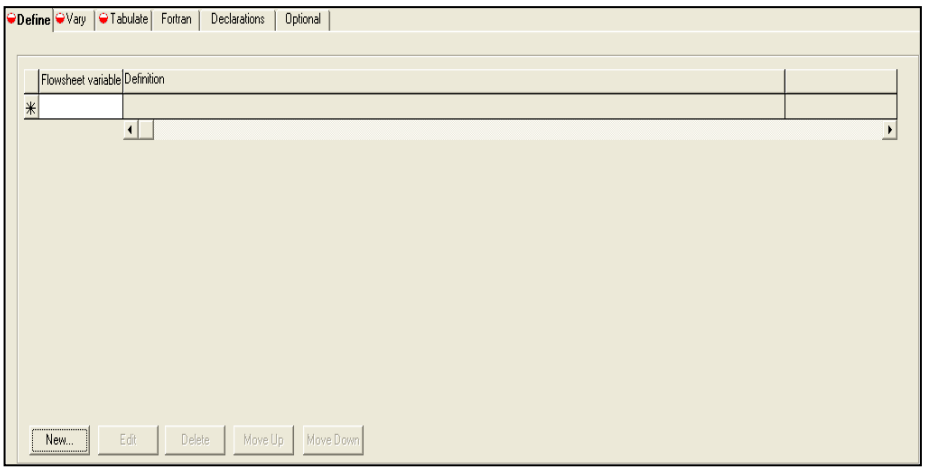


Figure 3.32 Define Sheet in Sensitivity

In order to identify the flow sheet variable in Define Sheet, firstly, a new variable is created by clicked the New button. A Create New Variable dialog box is seen as shown in Figure 3.33. In the dialog box, the name of the variable is entered in the Variable Name field and then OK button is clicked. Next, a Variable Definition Sheet with Category frame and Reference frame are seen as shown in Figure 3.34. In the Category frame, the option button is used to select the variable category. In the Reference frame, the variable type is selected from the list in the Type field. It will display the other fields necessary to complete the variable definition. Lastly, Close button is clicked in order to return to the Define Sheet.

Figure 3.33 Create New Variable Dialog Box

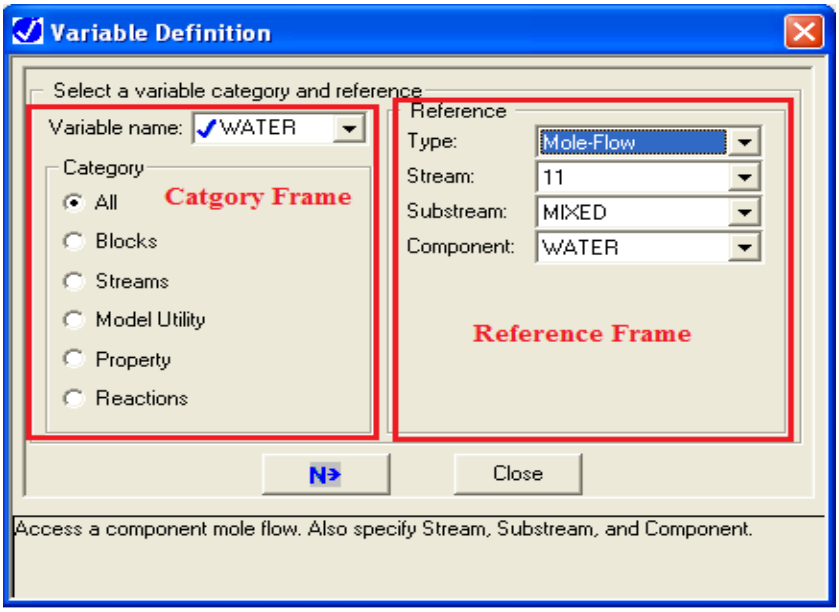


Figure 3.34 Variable Definition Sheet in Sensitivity Analysis

3.3.3 Step 3: Specify Manipulated/Varies Flow Sheet Variables

Vary Sheet as shown in Figure 3.35 is used to identify the flow sheet variables to vary in generating a table. The manipulated flow sheet variables can only vary block input variable, process feed stream variables, and other input variables. Besides that, it must specify the values, or a range of values, for the varied variables. In order to identify the manipulated variables, firstly, on the Sensitivity input form,

the Vary Sheet is clicked. A manipulated variable field is seen as shown in the red box of Figure 3.35. In the Manipulated Variable field, a variable type is selected and it will take the remaining fields necessary to uniquely identify the flow sheet variable.

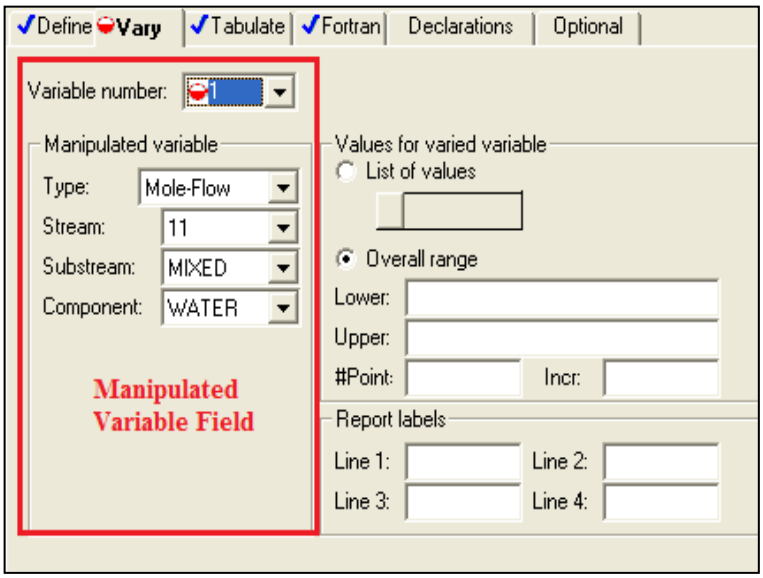


Figure 3.35 Manipulated Variable Field in Vary Sheet

3.3.4 Step 4: Specify Ranges for Manipulated/Varied Variables

Values for varied variable field as shown in Figure 3.36 are used to specify the ranges for manipulated variables. There are four type of ranges can be specify which are 1) list of values, 2) lower limit, upper limit, and number of equally spaced point (#Points), 3) lower limits, upper limits, and increment between point (Incr) and 4) labeling the varied variables for the report and the Result Summary Sheet.

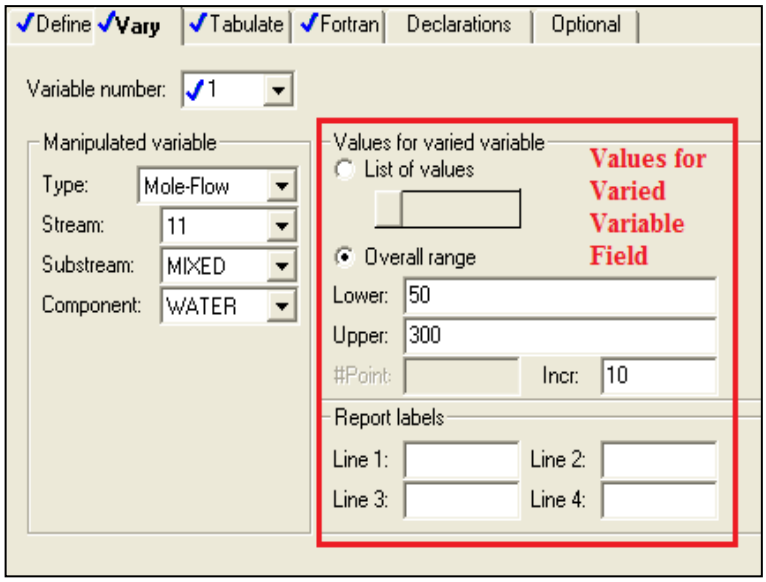


Figure 3.36 Values Varied Variable Field in Vary Sheet

3.3.5 Step 5: Defining Tabulated Variables

Tabulate Sheet as shown in Figure 3.37 is used to define the results required to be analysis and supplied column headings. In order to tabulate variables, firstly, in the Sensitivity Input form, the Tabulate Sheet is clicked. In the Column Number field, a column number is entered. In the Tabulated Variable or Expression field, a variable name or Fortran expression is entered. The Fortran statements as shown in Figure 3.38 is used to compute tabulated results and the varied variable range. It is needed only if functions are too complex to enter on these sheets. In order to executable Fortran statements on the Fortran sheet, firstly, on the Sensitivity Input form, the Fortran sheet is clicked. Then, the Fortran statements is entered.

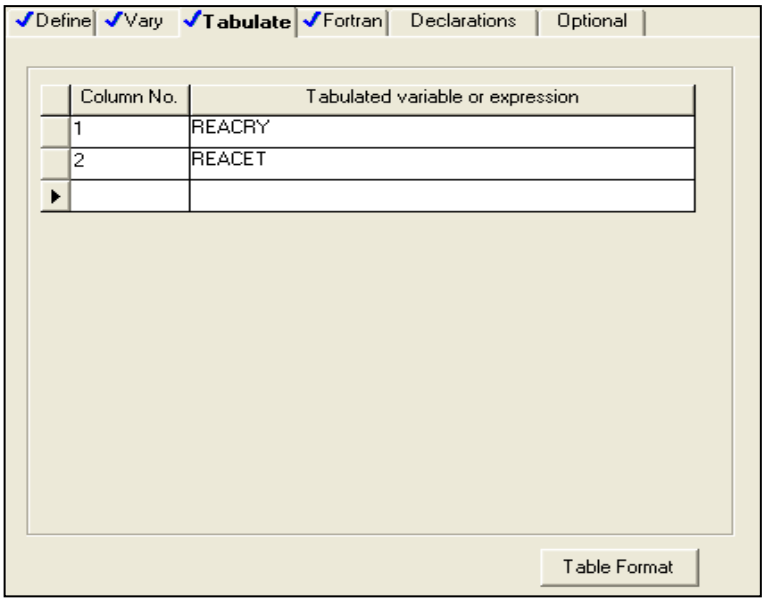


Figure 3.37 Tabulate Sheet in Sensitivity Analysis

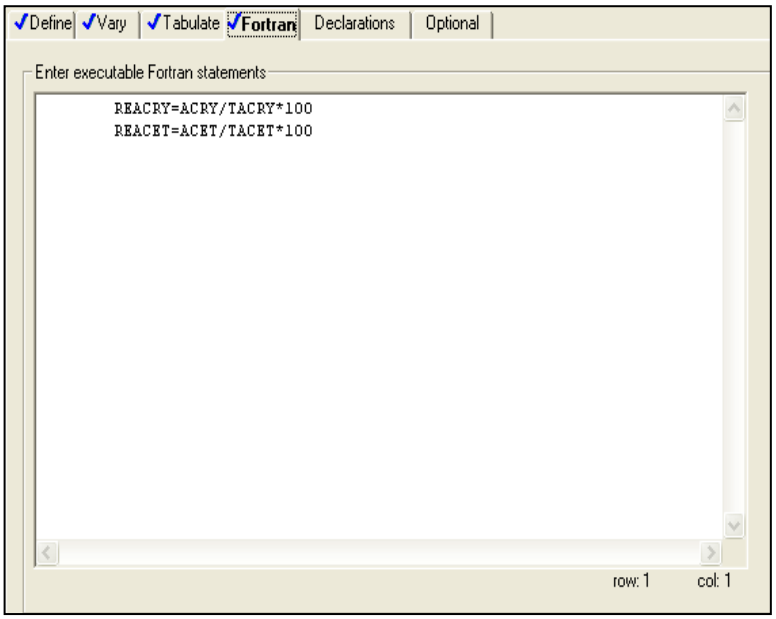


Figure 3.38 Fortran Sheet in Sensitivity Analysis

3.3.6 Step 6: Running the Simulation

After all the procedures of sensitivity analysis are done, the flow sheet has to be reinitialized in order to prevent the Aspen Plus using the previous results to precede the simulation. To do this, from the Run menu, the Reinitialize button is clicked and a dialog box of reinitialize is seen as shown in Figure 3.39. On the dialog box, Ok button is clicked twice in order for confirmation of reinitialize dialog box as shown in Figure 3.40.

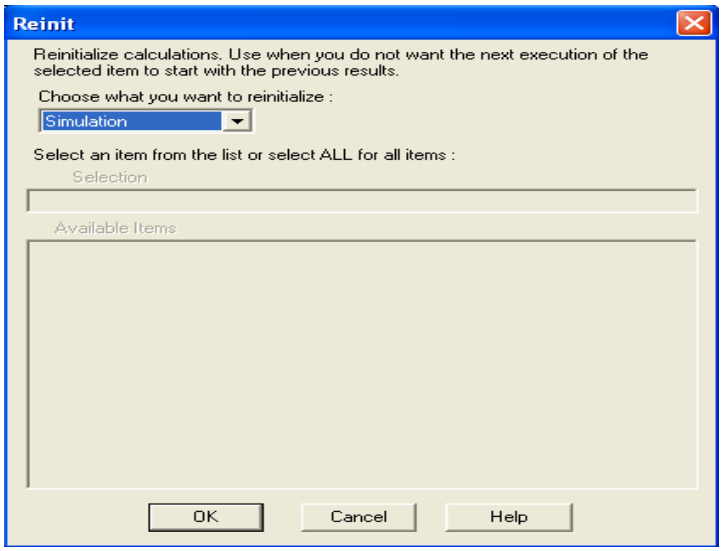


Figure 3.39 Reinitialize Dialog Box

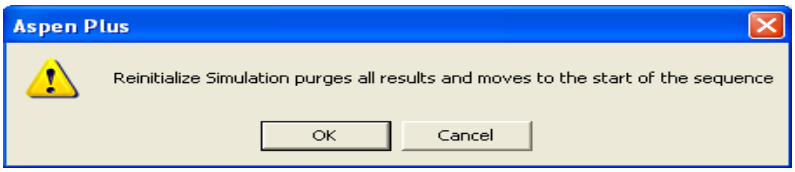


Figure 3.40 Confirmation of Reinitialize Dialog Box

3.3.7 Information for Each Sensitivity Block

The previous section is mention about the procedure how to carry out the sensitivity analysis in Aspen Plus software. In this acrylic acid plant, the sensitivity analysis is carried on each model which consists of reactor, flash drum, adsorption tower, liquid-liquid extractor, distillation column 1 and distillation column 2. There are totally eleven sensitivity analyses of the flow sheet. By using the sensitivity analysis, it determined the key operating or design variables of models and these design variables are shown in Table 3.3. All of these design variables are used as the manipulated variables respectively for each sensitivity block. In the Table 3.4, it shows that the flow sheet variables that used for each sensitivity block which is used in Fortran statement or tabulate variables.

Table 3.3 Design Variables for each Model

Models	Design Variables
Reactor	Temperature
Flash drum	Temperature and pressure
Absorption tower	Water flow rate
Liquid-liquid extractor	Diisopropyl-ether flow rate
Packed distillation column	Feed stage, reflux ratio, and re-boiler duty
Distillation Column	Feed stage, reflux ratio, and re-boiler duty

Table 3.4 Flow Sheet Variables of Each Sensitivity Block

Sensitivity Block	Flow Sheet Variables	Definition
R301-T	PROIN	Mole-Flow Stream=7 Substream=MIXED Component=PROPY-01
	ACRY	Mole-Flow Stream=8 Substream=MIXED Component=ACRY-01
T301-P/ T301-T	ACRY	Mole-Flow Stream=13 Substream=MIXED Component=ACRYL-01

Table 3.4 (Continued)

Sensitivity Block	Flow Sheet Variables	Definition
	TACRY	Mole-Flow Stream=9 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=13 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=9 Substream=MIXED Component=ACETI-01
T302-WAT	ACRY	Mole-Flow Stream=14 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=10 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=14 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=10 Substream=MIXED Component=ACETI-01
T303-DIISO	ACRY	Mole-Flow Stream=18 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=15 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=18 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=15 Substream=MIXED Component=ACETI-01
T304-FS/ T304-RR/ T304-RD	ACRY	Mole-Flow Stream=20 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=18 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=20 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=18 Substream=MIXED Component=ACETI-01
	DIISO	Mole-Flow Stream=19 Substream=MIXED Component=DIISO-01
	TDIISO	Mole-Flow Stream=18 Substream=MIXED Component=DIISO-01
T305-FS/ T305-RR/ T305-RD	ACRY	Mole-Flow Stream=22 Substream=MIXED Component=ACRYL-01
	TOTAL1	Stream-Var Stream=22 Substream=MIXED Variable=MOLE-FLOW
	ACET	Mole-Flow Stream=21 Substream=MIXED Component=ACETI-01
	TOTAL2	Stream-Var Stream=21 Substream=MIXED Variable=MOLE-FLOW

By using the sensitivity analysis, it found out the range of manipulated variables. The lower limit, upper limit and increment of manipulated variable for each sensitivity block are shown in Table 3.5. Each sensitivity block has their own tabulate variables to be monitored such as yield (reactor), recovery of acrylic acid, acetic acid and diisopropyl-ether (flash drum, absorption tower, liquid-liquid extractor, and distillation column 1) and purity of acrylic acid and acetic acid (distillation column 2). Fortran in sensitivity analysis is used to set the formula or statement for tabulate variable by using flow sheet variables. The column number, tabulate variables, and Fortran statement for each sensitivity block is shown in Table 3.6.

Table 3.5 Manipulated Variables, Lower Limit, Upper Limit and Increment for Each Sensitivity Block

Sensitivity Blok	Manipulated Variable	Lower Limit	Upper Limit	Increment
R301-T	Temperature	523K	638K	5
T301-P	Pressure	0.5atm	5.0atm	0.5
T301-T	Temperature	283K	328K	5
T302-WAT	Water Flow Rate	10kmol/hr	200kmol/hr	10
T303-DIISO	Diisopropyl-ether Flow Rate	50kmol/hr	1350kmol/hr	50
T304-FS	Feed Stage	1	10	1
T304-RR	Reflux Ratio	0.5	10	0.5
T304-RD	Re-boiler Duty	40000MJ/hr	300000MJ/hr	20000MJ/hr
T305-FS	Feed Stage	2	36	1
T305-RR	Reflux Ratio	1	15	1
T305-RD	Re-boiler Duty	200MJ/hr	3000MJ/hr	200MJ/hr

Table 3.6 Column Number, Tabulate Variables and Fortran Statement for Each Sensitivity Block

Sensitivity Block	Column Number	Tabulate Variables	Fortran Statement
R301-T	1	YIELD	YIELD = ACRY/PROIN
T301-P/ T301-T	1	REACRY	REACRY=ACRY/TACRY*100
	2	REACET	REACET=ACET/TACET*100
T302-WAT	1	REACRY	REACRY=ACRY/TACRY*100
	2	REACET	REACET=ACET/TACET*100
T303-DIISO	1	REACRY	REACRY=ACRY/TACRY*100
	2	REACET	REACET=ACET/TACET*100
T304-FS/ T304-RR/ T304-RD	1	REACRY	REACRY=ACRY/TACRY*100
	2	REACET	REACET=ACET/TACET*100
	3	REDIISO	REDIISO=DIISO/TDIISO*100
T305-FS/ T305-RR/ T305-RD	1	PUR1	PUR1=ACRY/TOTAL1*100
	2	PUR2	PUR2=ACET/TOTAL2*100

3.4 Optimization

After the simulation is started and the sensitivity analysis is performed, optimization can be preceded and it has totally six steps in Aspen Plus. A brief flow chart on optimization is shown in Figure 3.41.

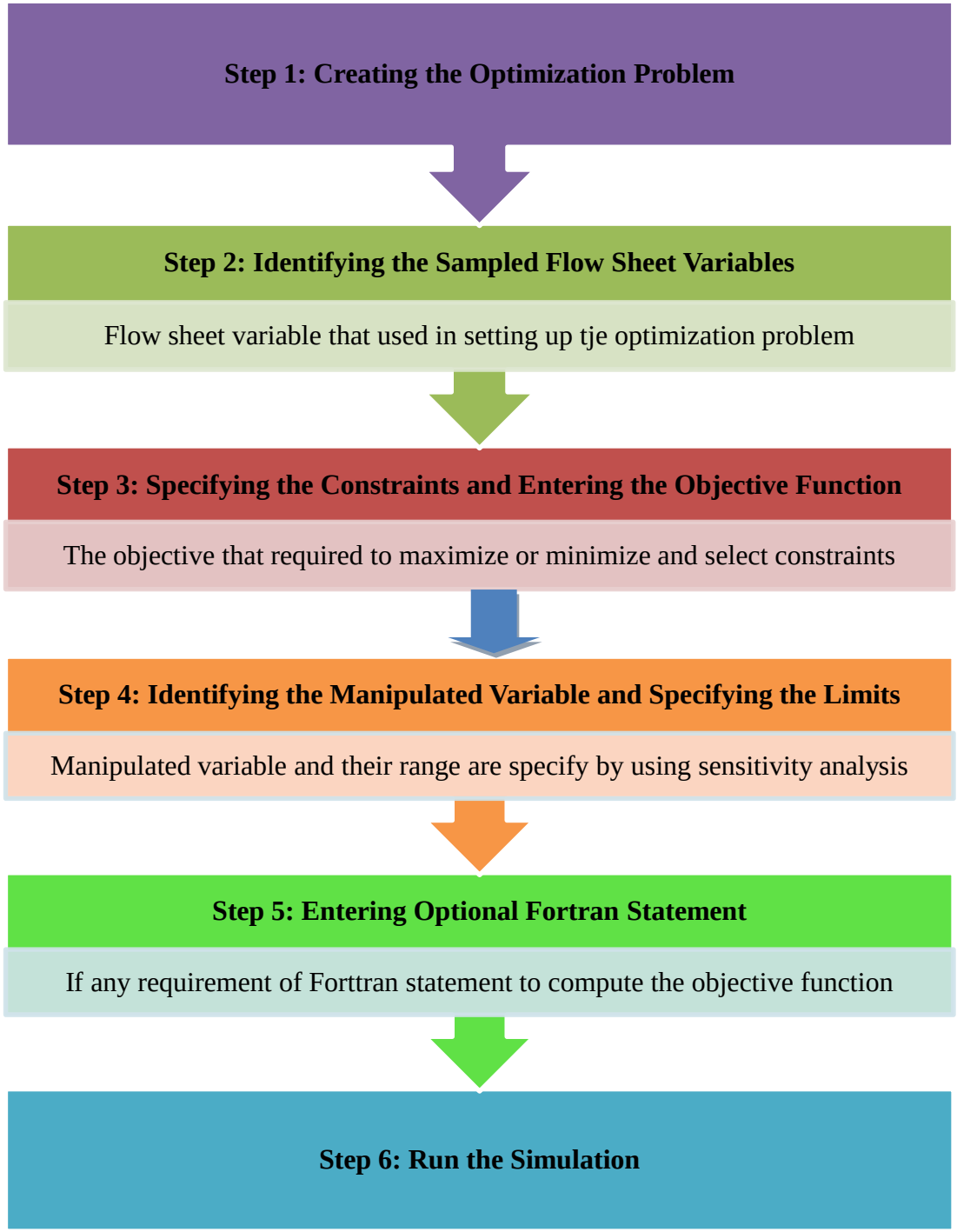


Figure 3.41 Brief Flow Chart on Optimization

3.4.1 Step 1: Creating the Optimization Problem

In order to create an optimization problem, firstly, from the Data menu, point to Model Analysis Tools and then Optimization button is clicked. In the Optimization Manager as shown in Figure 3.42, the New button is clicked. In the Create New ID dialog box as shown in Figure 3.43, an ID is entered and then Ok button is clicked.

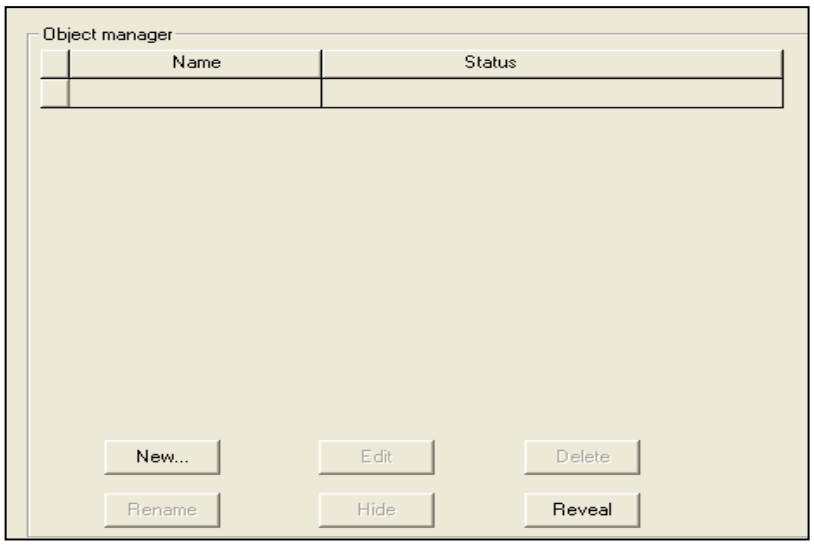


Figure 3.42 Constraint Object Manager

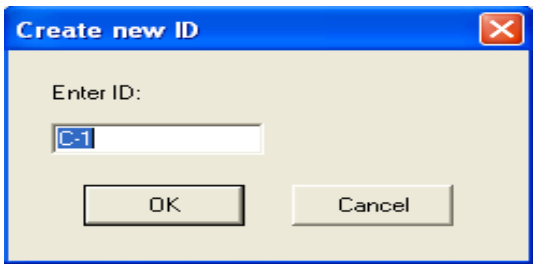


Figure 3.43 Create New ID Dialog Box

3.4.2 Step 2: Identifying the Sampled Flow Sheet Variables

Define sheet as shown in Figure 3.44 is used to identify a flow sheet variable and assign it a variable name. The variable is used for defining the objective function, specifying bounds for manipulated variables, or writing Fortran Statements. After completing a Define sheet, variables is specified on the Variable Definition dialog box. In order to create a new variable, firstly, the New button is clicked on the Define sheet. In the Create New Variable Dialog as shown in Figure 3.45, the name of the variable in the Variable Name field is entered. After clicked the Ok button, Category and Reference frame are seen in the Variable Definition dialog box as shown in Figure 3.46. In the Category frame, the option button is used to select the variable category. In the Reference frame, the variable type is selected from the list in the Type field. Lastly, Close button is clicked to return to the Define sheet.

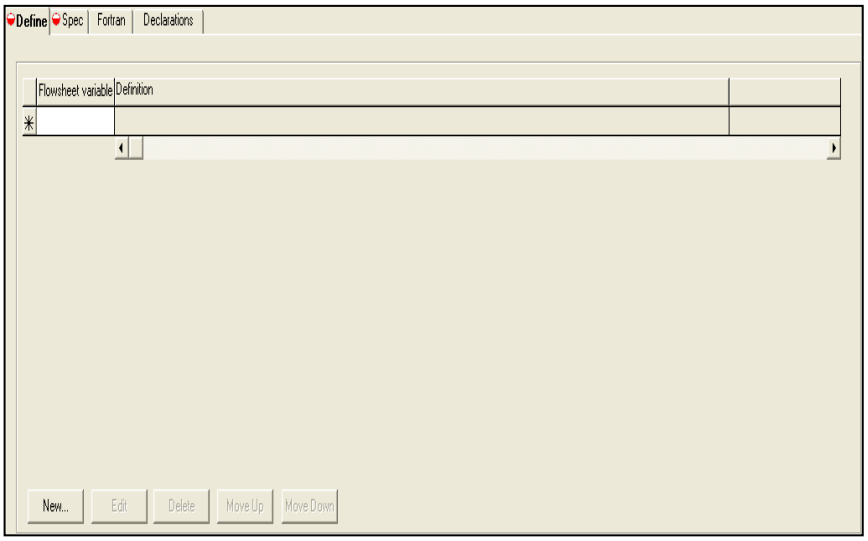


Figure 3.44 Define Sheet in Constraint

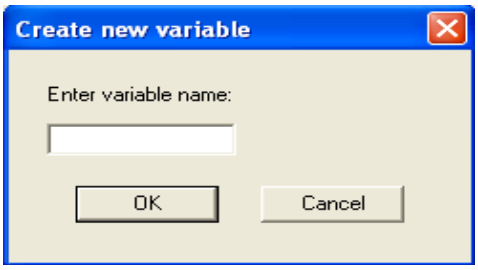


Figure 3.45 Create New Variable Dialog Box

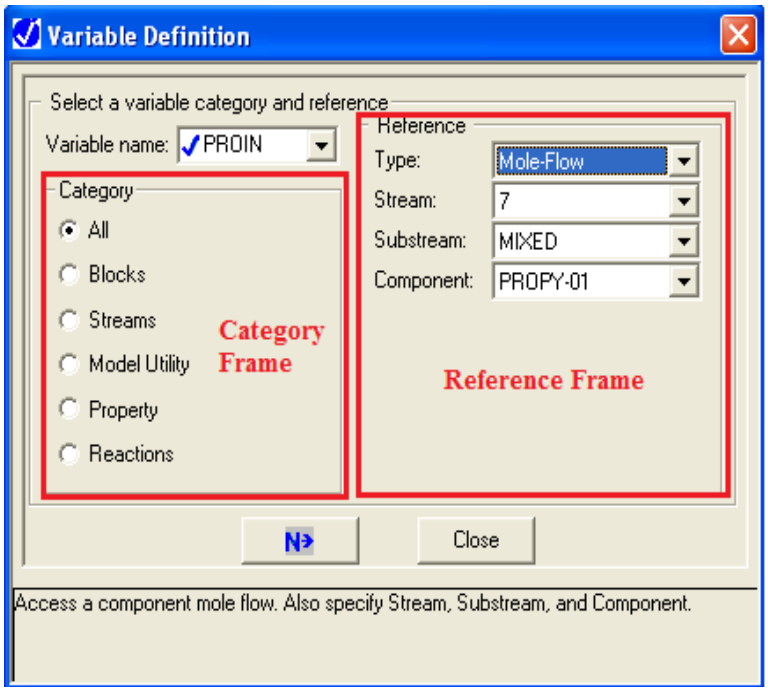


Figure 3.46 Variable Definition Sheet

3.4.3 Step 3: Specifying the Constraints and Entering the Objective Function

3.4.3.1 Specification of Constraints

Before running the optimization in Aspen Plus software, the equality or inequality of constraints has imposed or specified in the Model Analysis Tool. Equality constraints within an optimization are similar to design specifications and

the constraints can be any function of flow sheet variables computed using Fortran statement or in-line Fortran statements. Besides that, the tolerance of the constraints must be specified. A brief flow chart of specification of constraints is shown in Figure 3.47.

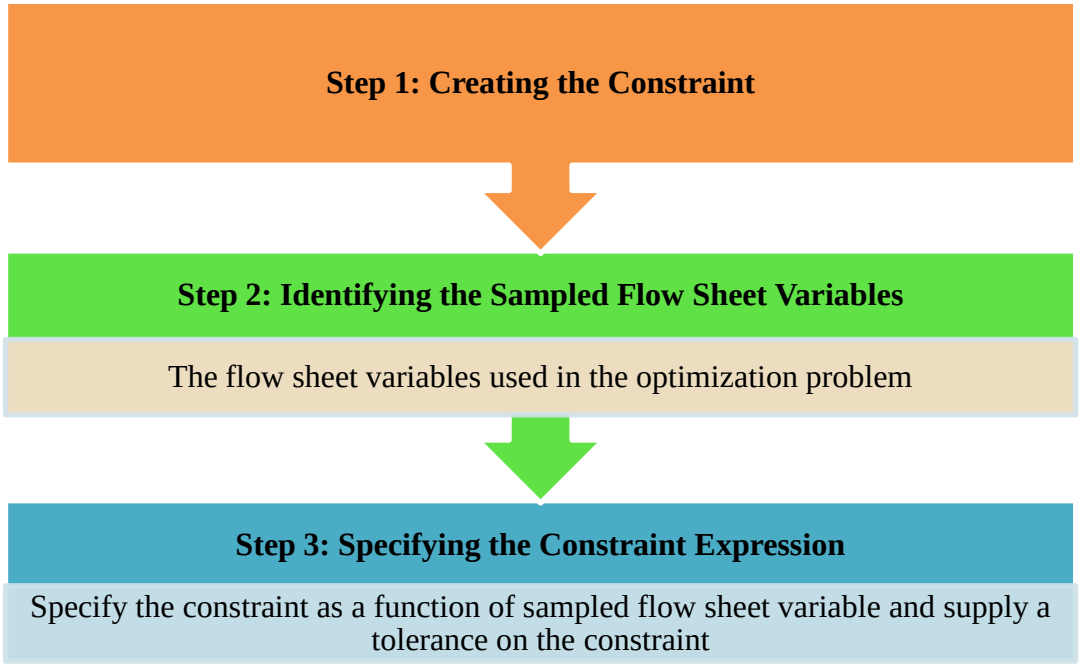


Figure 3.47 Brief Flow Chart of Specification of Constraints

3.4.3.2 Step 1: Creating the Constraint

In order to create the constraint, firstly, from the Data menu, point to Model Analysis Tools and the Constraint is clicked. In the Constraint Object Manager as shown in Figure 3.48, New button is clicked. In the Create New ID dialog Box as shown in Figure 3.49, an ID is entered and then Ok button is clicked.

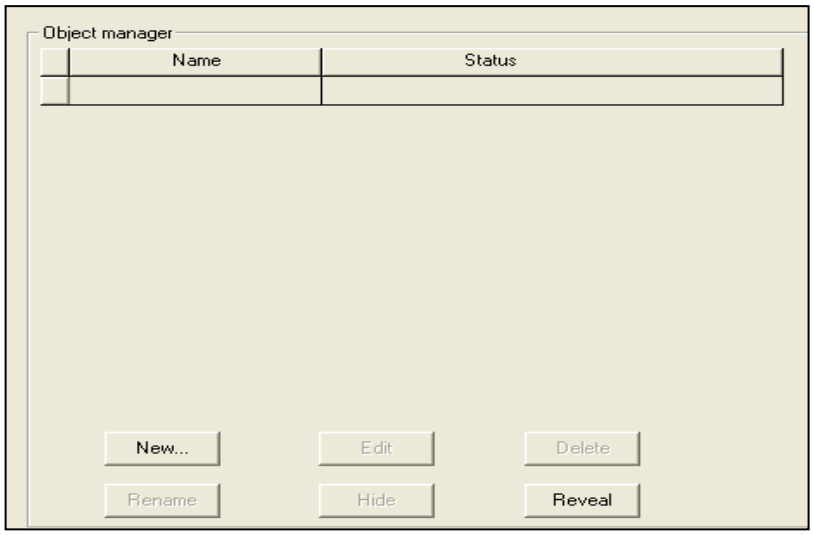


Figure 3.48 Constraint Object Manager

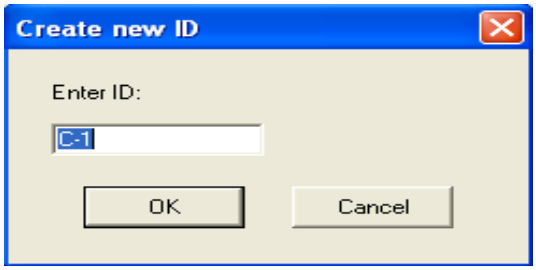


Figure 3.49 Create New ID Dialog Box

3.4.3.3 Step 2: Identifying the Sampled Flow Sheet Variables

Define sheet as shown in Figure 3.50 is used to identify a flow sheet variable and assign it a variable name. After completing a Define sheet, variables is specified on the Variable Definition dialog box. In order to create a new variable, firstly, the New button is clicked on the Define sheet. In the Create New Variable Dialog as shown in Figure 3.51, the name of the variable is entered in the Variable Name field. After clicked the Ok button, Category and Reference frame are seen in the Variable Definition dialog box as shown in Figure 3.52. In the Category frame, the option

button is used to select the variable category. In the Reference frame, the variable type is selected from the list in the Type field. Lastly, Close button is clicked to return to the Define sheet.

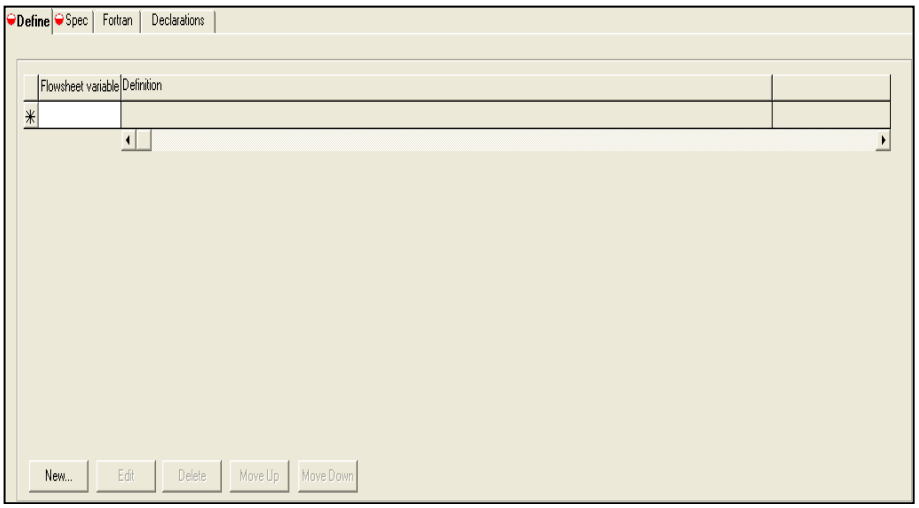


Figure 3.50 Define Sheet in Constraint

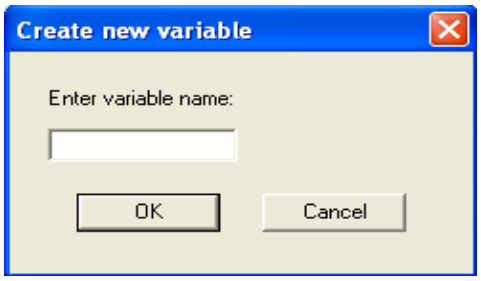


Figure 3.51 Create New Variable Dialog Box

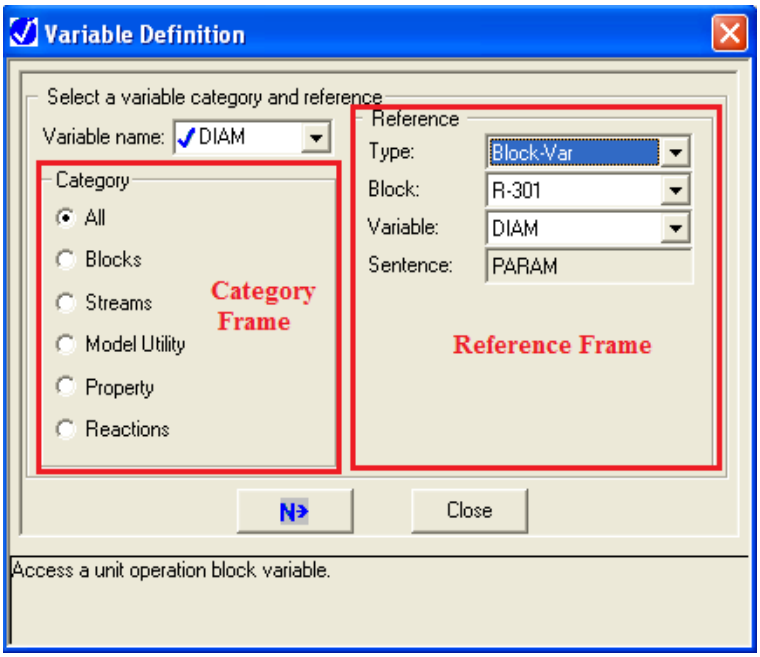


Figure 3.52 Variable Definition Sheet

3.4.3.4 Step 3: Specifying the Constraint Expression

The specification, type of constraints and tolerance had been specified in the Specification sheet. In order to specify the constraint, on the Constraint form, the Spec tab is clicked. A specification sheet is seen as shown in 3.53. In the specification fields, the variables that used in Constraint are entered and it can be the flow sheet variables or Fortran statements. Next, the type of constraints such as "equal to", "less than or equal to", or "greater than or equal to" is selected for the specification. On the Tolerance field, the constraint tolerance is entered as a constant or as a Fortran expression. If the constraint is a vector, the Vector Constraint box is checked, and the elements of the vector that should be used are specified.

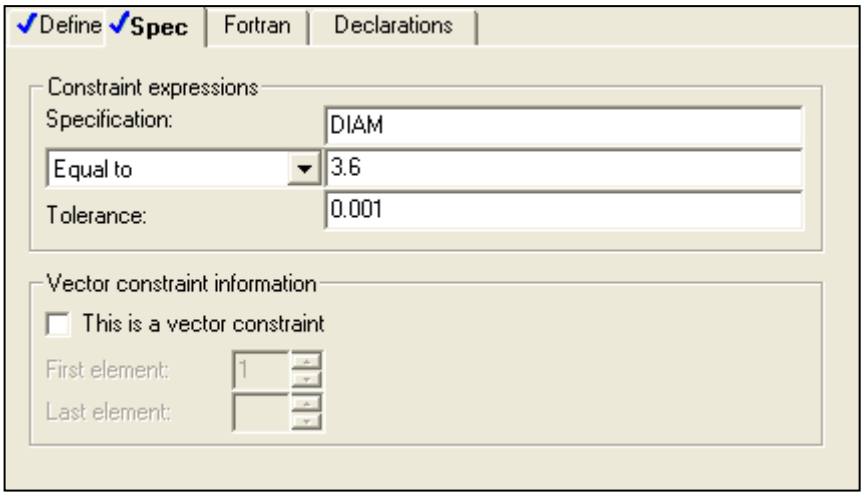


Figure 3.53 Specification Sheet of Constraint

3.4.3.5 Information of Each Constraint Block

The previous section is mentioned about the procedure how to carry out the constraint in optimization. There are totally sixteen constraints in the models which include reactor, flash drum, absorption tower, liquid-liquid extractor, distillation column 1, and distillation column 2. The constraints for each model are shown in Table 3.7 and flow sheet variables for constraint blocks are shown in Table 3.8.

Table 3.7 Constraints of Each Model

Models	Constraints
Reactor	Diameter, length, pressure drop, and number of tube
Flash Drum	Pressure, and temperature
Absorption Tower	Condenser duty, number of stage, and re-boiler duty
Liquid-liquid Extractor	Number of stage
Packed Distillation Column	Bottom rate, feed stage, and number of stage
Distillation Column	Bottom rate, feed stage, and number of stage

Table 3.8 Flow Sheet Variables for Each Constraint

Constraint Name	Flow Sheet Variables	Definition
R-DIAM	DIAM	Block-Var Block=R-301 Variable=DIAM Sentence=PARAM
R-LENGTH	LENGTH	Block-Var Block=R-301 Variable=LENGTH Sentence=PARAM
R-PD	PD	Block-Var Block=R-301 Variable=PDROP Sentence=PARAM
R-TUBE	TUBE	Block-Var Block=R-301 Variable=NTUBE Sentence=PARAM
T301-CT	TEM	Block-Var Block=T-301 Variable=TEMP Sentence=PARAM
T301-CP	PRES	Block-Var Block=T-301 Variable=PRES Sentence=PARAM
T302-CD	CD	Block-Var Block=T-302 Variable=COND-DUTY Sentence=RESULTS ID1=1
T302-NS	NS	Block-Var Block=T-302 Variable=CC-NSEGMENT Sentence=COL-CONFIG ID1=1
T302-RD	RD	Block-Var Block=T-302 Variable=REB-DUTY Sentence=RESULTS ID1=1
T303-NS	NS	Block-Var Block=T-303 Variable=NSTAGE Sentence=PARAM
T304-BR	BR	Block-Var Block=T-304 Variable=MOLE-B Sentence=COL-SPECS
T304-FS	FS	Block-Var Block=T-304 Variable=FEED-STAGE Sentence=FEEDS ID1=18
T304-NS	NS	Block-Var Block=T-304 Variable=NSTAGE Sentence=PARAM
T305-BR	BR	Block-Var Block=T-305 Variable=MOLE-B Sentence=COL-SPECS
T305-FS	FS	Block-Var Block=T-304 Variable=FEED-STAGE Sentence=FEEDS ID1=18
T305-NS	NS	Block-Var Block=T-305 Variable=NSTAGE Sentence=PARAM

Table 3.9 shows that the specification, type of Constraint, and tolerance for each constraint block. Lastly, the constraint blocks had been ensured to be selected on the Optimization Objective and Constraint sheet in order to carry out the optimization.

Table 3.9 Specifications, Type of Constraint, and Tolerance for Each Constraint

Constraint Name	Specification	Type of Constraint	Tolerance
R-DIAM	DIAM	Equal to 3.6	0.001
R-LENGTH	LENGTH	Equal to 10	0.001
R-PD	PD	Equal to 0	0.001
R-TUBE	TUBE	Equal to 420	0.001
T301-CT	TEM	Equal to 313.15	0.001
T301-CP	PRES	Equal to 2.36	0.001
T302-CD	CD	Equal to 0	0.001
T302-NS	NS	Equal to 15	0.001
T302-RD	RD	Equal to 0	0.001
T303-NS	NS	Equal to 15	0.001
T304-BR	BR	Equal to 96	0.001
T304-FS	FS	Equal to 4	0.001
T304-NS	NS	Equal to 15	0.001
T305-BR	BR	Equal to 90	0.001
T305-FS	FS	Equal to 23	0.001
T305-NS	NS	Equal to 36	0.001

3.4.3.6 Selecting the Constraints

If any constraints are associated with the optimization, defined them after specified the Objective Function because it is influenced the result of optimization. In order to enter the objective function for the optimization problem, firstly, on the optimization form, the Objective & Constraints tab is clicked. The Objective & Constraints sheet is seen as shown in Figure 3.54. In the Objective Function field, either Maximize or Minimize is selected and the targeted variable or Fortran expression is entered. Each of the models had different Objective Function. Next, the constraints are selected that to be associated with the optimization by using the arrow buttons to move them from the available Constraints list to the Selected Constraints list.

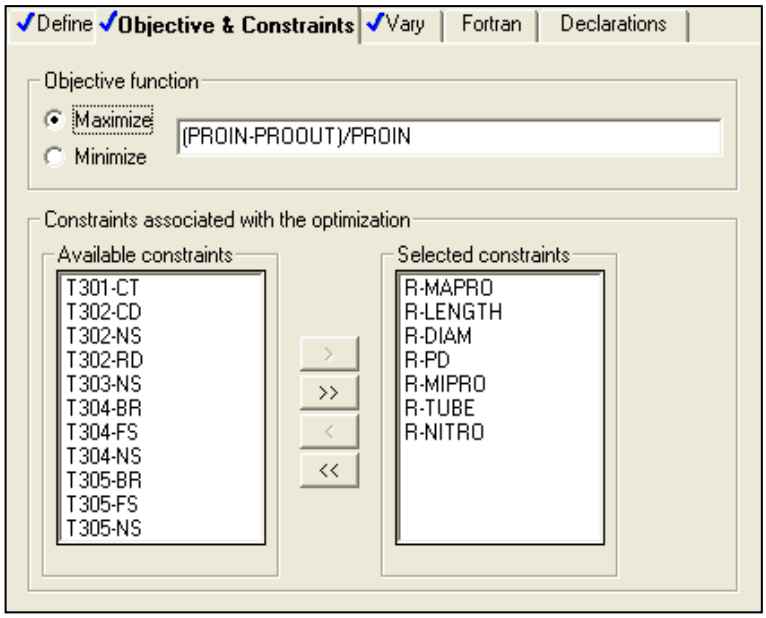


Figure 3.54 Objective & Constraints Sheet

3.4.4 Step 4: Identifying the Manipulated Variable and Specifying the Limits

The Vary sheet in the optimization is used to identify the manipulated variables and specify their limits. The limits for manipulated variable can be constants or function of flow sheet variables. In order to identify the manipulated variable and specify the limits, on the Optimization form, the Vary tab is clicked. The Vary sheet is seen as shown in the Figure 3.55. In the Variable Number field, the down arrow is clicked and then <new> is selected. In the type field, a variable type is selected and the remaining field is filled. In the Manipulated Variable Limits field, the lower and upper limits are entered by a constant value or Fortran expression. The decision variables for the report and Results form are labeled by using the Line 1 to Line 4 fields. The step size and maximum step size is entered in the Steps Size Parameters field.

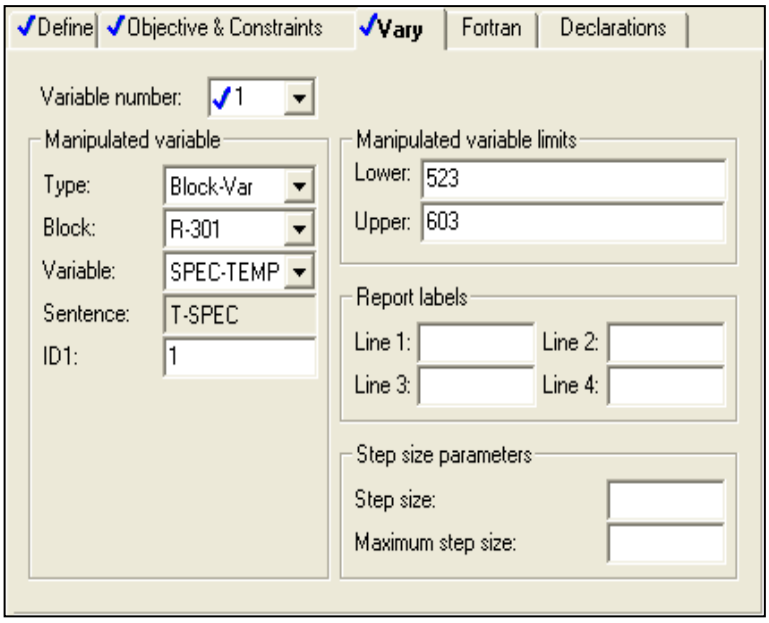


Figure 3.55 Vary Sheet in Optimization

3.4.5 Step 5: Entering Optional Fortran Statement

The Fortran statement is used to compute the optimization objective terms or manipulated variable limits. In order to enter executable Fortran statements on the Fortran sheet, firstly, on the Optimization form, the Fortran tab is clicked. The Fortran sheet is seen as shown in Figure 3.56 and then the Fortran statements is entered for each optimization block.

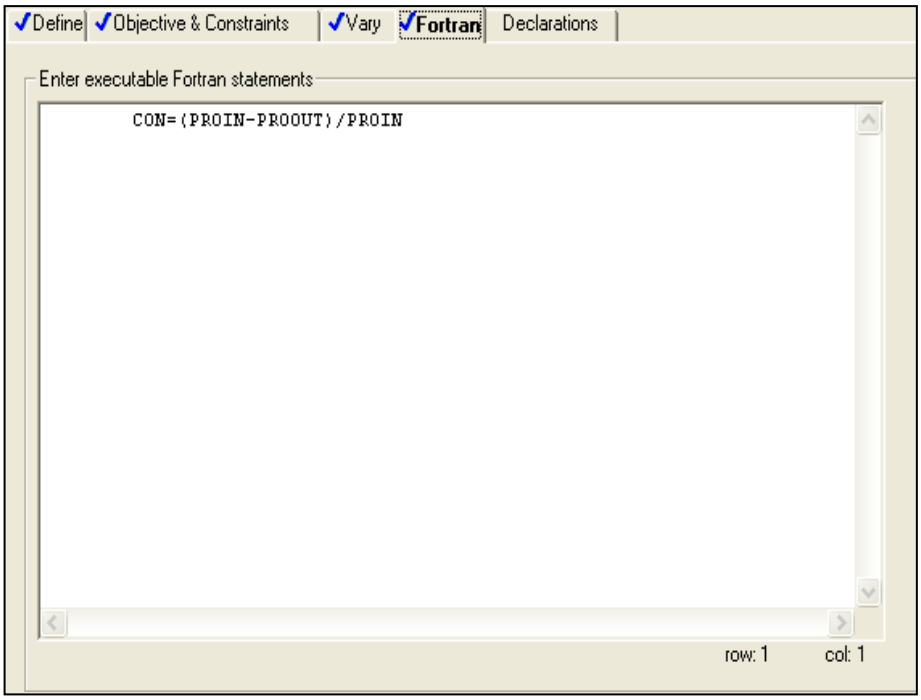


Figure 3.56 Fortran Sheet in Optimization

3.4.6 Step 6: Running the Simulation

After all the procedures of optimization are done, the same procedures for running the simulation in sensitivity section were used. In order to reinitialize the flow sheet, from the Run menu, the Reinitialize is clicked and a dialog box is seen as shown in Figure 3.39. On the dialog box, Ok button is clicked twice for confirmation of reinitialize dialog box as shown in Figure 3.40.

3.4.7 Information for Each Optimization Block

The previous section is mentioned about the procedures how to carry out the optimization in Aspen Plus software. There are totally nine optimization blocks in

the flow sheet. The optimization is carry on each models which are reactor, flash drum, absorption tower, liquid-liquid extractor, distillation column 1 and distillation column 2. The optimization parameters for each model are shown in Table 3.10 and flow sheet variables for each optimization blocks are shown in Table 3.11.

Table 3.10 Parameters of Optimization for Each Model

Models	Parameters
Reactor	Temperature
Flash drum	Temperature and pressure
Absorption tower	Water flow rate
Liquid-liquid extractor	Diisopropyl-ether flow rate
Packed distillation column	Feed stage, reflux ratio, and re-boiler duty
Distillation Column	Feed stage, reflux ratio, and re-boiler duty

Table 3.11 Flow Sheet Variables of Each Optimization Block

Sensitivity Block	Flow Sheet Variables	Definition
R301-T	PROIN	Mole-Flow Stream=7 Substream=MIXED Component=PROPY-01
	ACRY	Mole-Flow Stream=8 Substream=MIXED Component=ACRY-01
T301-PRE/ T301-TEM	ACRY	Mole-Flow Stream=13 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=9 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=13 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=9 Substream=MIXED Component=ACETI-01
T302-WAT	ACRY	Mole-Flow Stream=14 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=10 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=14 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=10 Substream=MIXED Component=ACETI-01

Table 3.11 (Continued)

Sensitivity Block	Flow Sheet Variables	Definition
T303-DIISO	ACRY	Mole-Flow Stream=18 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=15 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=18 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=15 Substream=MIXED Component=ACETI-01
T304-RR/ T304-RD	ACRY	Mole-Flow Stream=20 Substream=MIXED Component=ACRYL-01
	TACRY	Mole-Flow Stream=18 Substream=MIXED Component=ACRYL-01
	ACET	Mole-Flow Stream=20 Substream=MIXED Component=ACETI-01
	TACET	Mole-Flow Stream=18 Substream=MIXED Component=ACETI-01
	DIISO	Mole-Flow Stream=19 Substream=MIXED Component=DIISO-01
	TDIISO	Mole-Flow Stream=18 Substream=MIXED Component=DIISO-01
T305-RR/ T305-RD	ACRY	Mole-Flow Stream=22 Substream=MIXED Component=ACRYL-01
	TOTAL1	Stream-Var Stream=22 Substream=MIXED Variable=MOLE-FLOW
	ACET	Mole-Flow Stream=21 Substream=MIXED Component=ACETI-01
	TOTAL2	Stream-Var Stream=21 Substream=MIXED Variable=MOLE-FLOW

The Objective Function and Constraints of each optimization blocks are shown in the Table 3.12. Each manipulated variables and range of limits of optimization blocks are specified by the sensitivity analysis. Table 3.13 shows that the manipulated variables, lower limit and upper limit for each optimization block. Fortran in optimization is used to setting the formula or statement of yield, recovery and purity of the desired products. Fortran statement for each optimization block are shown in the Table 3.14.

Table 3.12 Objective Function and Selected Constraints in Optimization

Optimization Block	Objective Function	Selected Constraints
R301-T	Maximize: YIELD	R-LENGTH, R-DIAM, R-PD, R-TUBE
T301-PRE	Maximize: REACRY+REACET	T301-CT
T301-TEM	Maximize: REACRY+REACET	T301-CP
T302-WAT	Maximize: REACRY+REACET	T302-CD, T302-RD, T302-NS
T303-DIS	Maximize: REACRY+REACET	T303-NS
T304-RR	Maximize: REACRY+REACET	T304-NS, T304-BR, T304-FS
T304-RD	Maximize: REACRY+REACET	T304-NS, T304-BR, T304-FS
T305-RR	Maximize: PUR1+PUR2	T305-NS, T305-BR, T305-FS
T305-RD	Maximize: PUR1+PUR2	T305-NS, T305-BR, T305-FS

Table 3.13 Manipulated Variable and Range Limit for Each Optimization Block

Sensitivity Blok	Manipulated Variable	Lower Limit	Upper Limit
R301-T	Temperature	523K	638K
T301-P	Pressure	1.0atm	5.0atm
T301-T	Temperature	283K	328K
T302-WAT	Water Flow Rate	50kmol/hr	200kmol/hr
T303-DIISO	Diisopropyl-ether Flow Rate	500kmol/hr	1350kmol/hr
T304-RR	Reflux Ratio	0.5	10
T304-RD	Re-boiler Duty	40000MJ/hr	300000MJ/hr
T305-RR	Reflux Ratio	10	15
T305-RD	Re-boiler Duty	50MJ/hr	3000MJ/hr

Table 3.14 Fortran Statement for Each Optimization Block

Optimization Block	Fortran Statement
R301-T	YIELD = ACRY/PROIN
T301-P/ T301-T	REACRY=ACRY/TACRY*100
	REACET=ACET/TACET*100
T302-WAT	REACRY=ACRY/TACRY*100
	REACET=ACET/TACET*100
T303-DIISO	REACRY=ACRY/TACRY*100
	REACET=ACET/TACET*100
T304-RR/ T304-RD	REACRY=ACRY/TACRY*100
	REACET=ACET/TACET*100
	REDIISO=DIISO/TDIISO*100
T305-RR/ T305-RD	PUR1=ACRY/TOTAL1*100
	PUR2=ACET/TOTAL2*100

3.5 Summary

This study is carried out on the optimization on acrylic acid plant by using the Aspen Plus software. The methodology is divided into three main phases: Steady state simulation of acrylic acid plant; Sensitivity analysis; Optimization. The optimum conditions for each units or models are obtained, hence desired quality of the products is achieved.

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Introduction

In this chapter, which is on results and discussions, all the simulation and optimization results were tabulated and analyzed. This chapter was divided into two main phases which are Phase I: steady state simulation and Phase II: Optimization. In Phase I, the results of simulation were tabulated. In Phase II, it was detailed out into formulation of optimization problem, data analysis, discussion and optimum condition decision.

4.2 Phase I: Steady State Simulation of Acrylic Acid Plant

In this study, the acrylic acid plant was simulated by using Aspen Plus and the flow sheet is shown in Figure 4.1. After simulation was performed, the simulation data is shown in Table 4.1.

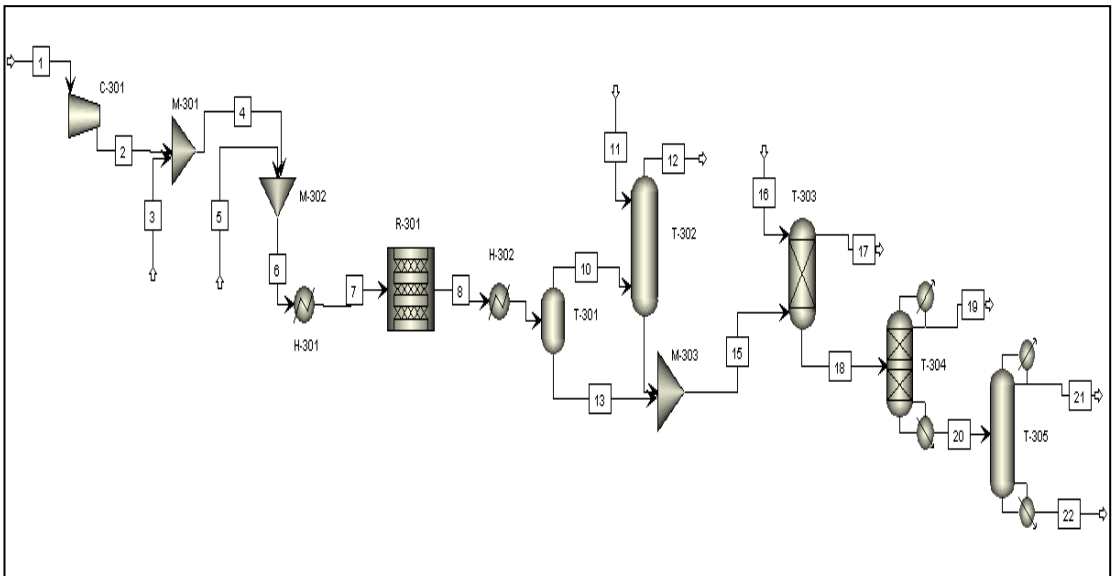


Figure 4.1 Flow Sheet for the production of Acrylic Acid Plant in Aspen Plus

Table 4.1 Simulation Data of Acrylic Acid Plant

	1	2	3	4	5	6
Temperature, ℃	25.00	285.42	159.00	225.79	25.00	201.05
Pressure, bar	1.00	5.00	6.00	5.00	11.50	5.00
Mole Flow kmol/h						
PROPY-01	0.00	0.00	0.00	0.00	127.00	127.00
NITRO-01	1056.70	1056.70	0.00	1056.70	0.00	1056.70
OXYGE-01	280.90	280.90	0.00	280.90	0.00	280.90
CARBO-01	0.00	0.00	0.00	0.00	0.00	0.00
WATER	25.30	25.30	992.30	1017.60	0.00	1017.60
ACETI-01	0.00	0.00	0.00	0.00	0.00	0.00
ACRYL-01	0.00	0.00	0.00	0.00	0.00	0.00
DIISO-01	0.00	0.00	0.00	0.00	0.00	0.00
Total Flow, kmol/h	1362.90	1362.90	992.30	2355.20	127.00	2482.20

Table 4.1 (Continued)

	7	8	9	10	11	12
Temperature, ℃	310.00	310.00	40.00	40.00	25.00	27.76
Pressure, bar	4.30	4.01	1.01	2.40	5.07	1.00
Mole Flow kmol/h						
PROPY-01	127.00	14.23	14.23	11.37	0.00	11.26
NITRO-01	1056.70	1056.70	1056.70	1051.19	0.00	1051.07
OXYGE-01	280.90	51.58	51.58	50.90	0.00	50.89
CARBO-01	0.00	60.17	60.17	55.79	0.00	55.69
WATER	1017.60	1166.12	1166.12	35.34	141.00	45.19
ACETI-01	0.00	6.54	6.54	0.09	0.00	0.00
ACRYL-01	0.00	88.35	88.35	1.40	0.00	0.00
DIISO-01	0.00	0.00	0.00	0.00	0.00	0.00
Total Flow, kmol/h	2482.20	2443.69	2443.69	1206.08	141.00	1214.10

Table 4.1 (Continued)

	13	14	15	16	17	18
Temperature, ℃	40.00	27.93	38.76	40.00	41.08	40.74
Pressure, bar	2.40	1.00	2.40	2.80	2.41	2.41
Mole Flow kmol/h						
PROPY-01	2.86	0.11	2.97	0.00	0.01	2.96
NITRO-01	5.51	0.12	5.63	0.00	0.01	5.62
OXYGE-01	0.68	0.01	0.69	0.00	0.00	0.69
CARBO-01	4.38	0.09	4.48	0.00	0.01	4.47
WATER	1130.78	131.16	1261.93	198.70	1327.61	133.02
ACETI-01	6.45	0.09	6.54	0.00	0.02	6.53
ACRYL-01	86.95	1.40	88.35	0.00	0.00	88.35
DIISO-01	0.00	0.00	0.00	1299.80	4.02	1295.78
Total Flow, kmol/h	1237.61	132.98	1370.59	1498.50	1331.68	1537.41

Table 4.1 (Continued)

	19	20	21	22
Temperature, ℃	35.22	64.28	40.56	78.83
Pressure, bar	0.10	0.10	0.10	0.10
Mole Flow kmol/h				
PROPY-01	2.96	0.00	0.00	0.00
NITRO-01	5.62	0.00	0.00	0.00
OXYGE-01	0.69	0.00	0.00	0.00
CARBO-01	4.47	0.00	0.00	0.00
WATER	133.02	0.00	0.00	0.00
ACETI-01	0.09	6.44	6.41	0.03
ACRYL-01	0.11	88.24	0.27	87.97
DIISO-01	1294.46	1.32	1.32	0.00
Total Flow, kmol/h	1441.41	96.00	8.00	88.00

One of the objectives of this study is to simulate a production of acrylic acid process. Hence, comparison between reference data and simulation results is not being considered. The final production rate of acrylic acid and acetic acid is mostly similar with the reference values, hence this simulation of acrylic acid production process is acceptable.

4.3 Optimization of Acrylic Acid Plant

4.3.1 Reactor (R-301)

4.3.1.1 Formulation of Optimization Problem (R-301)

Reactor is the heart of a chemical process plant. A favorable operating condition of reactor can maximize the yield of desired components and hence reduce the purification costs. Since oxidation of propylene is parallel chemical reactions,

therefore yield of acrylic acid and total conversion of propylene is influenced by the operating conditions. The optimization objective for the reactor is to obtain an optimum temperature to maximize the yield of acrylic acid. Therefore, temperature of reactor is taken as the manipulated variable while yield of acrylic acid as a measured variable. The constant variables present are pressure and inlet mole fraction of propylene.

4.3.1.2 Result and Discussion (R-301)

The result of sensitivity analysis of reactor is shown in Table 4.2. Figure 4.2 shows the graph of yield of acrylic acid versus the temperature of reactor. Figure 4.3 shows the optimization data of the reactor.

Table 4.2 Sensitivity Analysis Data of Reactor (R-301)

Temperature, ℃	Yield, Y	Temperature, ℃	Yield, Y
250	0.156834	310	0.693368
255	0.17982	315	0.772839
260	0.205646	320	0.761588
265	0.234596	325	0.750139
270	0.266972	330	0.738526
275	0.303101	335	0.726631
280	0.34333	340	0.710126
285	0.388031	345	0.687386
290	0.4376	350	0.66512
295	0.492457	355	0.643503
300	0.553051	360	0.621816
305	0.619854	365	0.600895

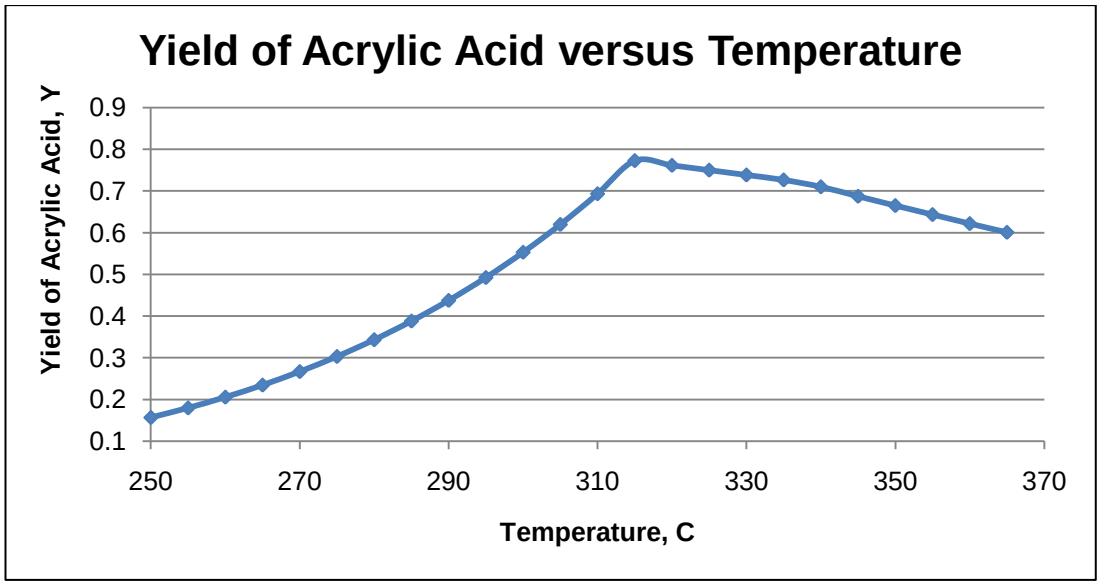


Figure 4.2 Yield of Acrylic Acid versus Temperature of Reactor (R-301)

```
OPTIMIZATION: R301
------------------

   SAMPLED VARIABLES:
     PROIN     : PROPY-01MOLEFLOW IN STREAM 7 SUBSTREAM MIXED
     ACRY      : ACRYL-01MOLEFLOW IN STREAM 8 SUBSTREAM MIXED

   FORTRAN STATEMENTS:
           YIELD=ACRY/PROIN

   OBJECTIVE FUNCTION:
     MAXIMIZE YIELD
     FINAL OBJECTIVE FUNCTION VALUE =            0.77254

   CONSTRAINTS: R-MAPRO    R-LENGTH  R-DIAM     R-PD       R-MIPRO
                R-TUBE     R-NITRO

   MANIPULATED VARIABLES:
     VARY      : SENTENCE=T-SPEC VARIABLE=TEMP ID1=1 IN UOS BLOCK R-301
     LOWER LIMIT =          523.000                      K
     UPPER LIMIT =          683.000                      K
     FINAL VALUE =          588.150                      K

   VALUES OF ACCESSED FORTRAN VARIABLES:
     VARIABLE       VALUE AT START      FINAL VALUE     UNITS
                      OF LOOP
     --------       --------------      -----------     -----
     PROIN            127.000             127.000       KMOL/HR
     ACRY             98.1130             95.2408       KMOL/HR
 ASPEN PLUS   PLAT: WIN32     VER: 11.1                    12/28/2012  PAGE 10
                              ACRYLIC ACID PLANT
                               FLOWSHEET SECTION
```

Figure 4.3 Optimization Data of Reactor (R-301)

After sensitivity analysis was carried out, the suitable range of temperature is varied from 250 ℃ to 365 ℃. From the Figure 4.2, the yield of acrylic acid depends on the operating temperature of reactor. As the temperature increased, the yield of acrylic acid is also increased but when the temperature is more than 315 ℃, the yield

starts to decreased linearly. Hence, the optimum temperature for maximum yield of acrylic acid is around 315℃. From Figure 4.3, in order to obtain the maximum yield of acrylic acid (0.77254), the final value of temperature is at 588.15K or 315℃. Therefore, 315℃ is the optimum temperature for the reactor.

4.3.2 Flash Drum (T-301)

4.3.2.1 Formulation of Optimization Problem (T-301)

The function of flash drum is to separate gases or vapor phase and acids in liquid phase. The liquid form of acids is separated out at the bottom outlet stream of flash drum and the separation efficiency depends on the operating pressure and temperature. Hence, optimization objective of flash drum is to maximize the recovery of acrylic acid and acetic acid at a minimum cost of operating conditions. Therefore, temperature and pressure of reactor are the manipulated variables, whereas, percentage of recovery of acrylic acid and acetic acid as the measured variables. The constant variables present are feed flow rate and size of flash drum.

4.3.2.2 Result and Discussion (T-301)

The result of sensitivity analysis for flash drum is shown in Table 4.3. The Figure 4.4 and Figure 4.5 show the graphs of recovery of acrylic acid and acetic acid

versus operating pressure with different temperature respectively. Figure 4.6 and 4.7 show the optimization data of flash drum with different optimization parameters.

Table 4.3 Sensitivity Analysis Data of Flash Drum (T-301)

Pressure, atm	10 ℃		25 ℃		40 ℃	
	REACRY	REACET	REACRY	REACET	REACRY	REACET
0.5	98.88	98.86	96.77	96.94	91.07	91.96
1	99.46	99.43	98.46	98.53	95.98	96.42
1.5	99.64	99.62	98.99	99.03	97.42	97.69
2	99.74	99.72	99.25	99.27	98.10	98.29
2.5	99.79	99.77	99.41	99.42	98.50	98.64
3	99.83	99.81	99.51	99.51	98.76	98.87
3.5	99.85	99.83	99.58	99.58	98.95	99.03
4	99.87	99.85	99.64	99.63	99.08	99.15
4.5	99.89	99.87	99.68	99.67	99.19	99.24
5	99.90	99.88	99.71	99.70	99.27	99.32

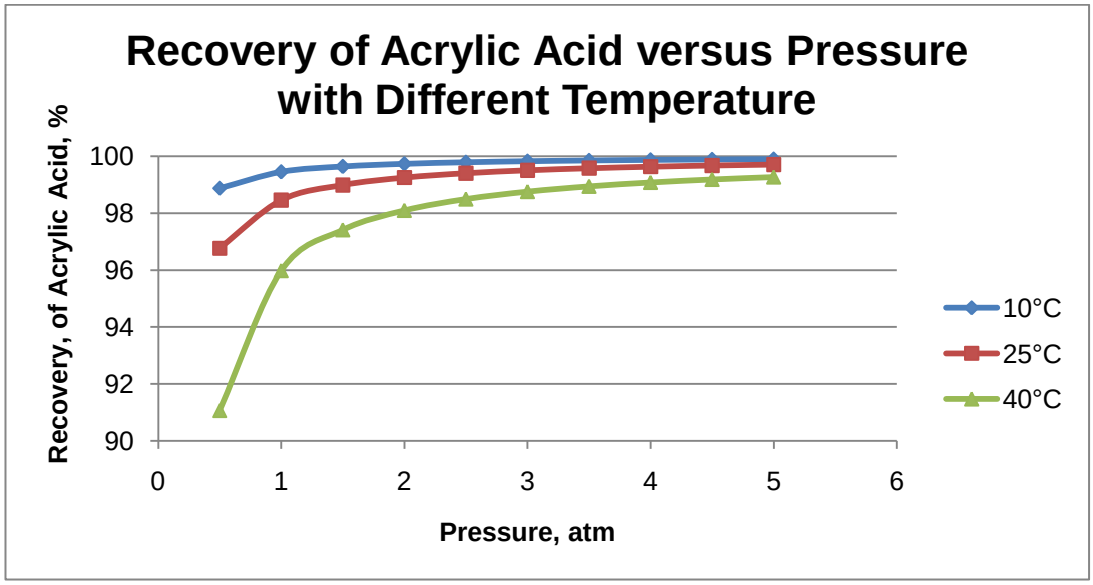


Figure 4.4 Recovery of Acrylic Acid versus Pressure with Different Temperature at Flash Drum (T-301)

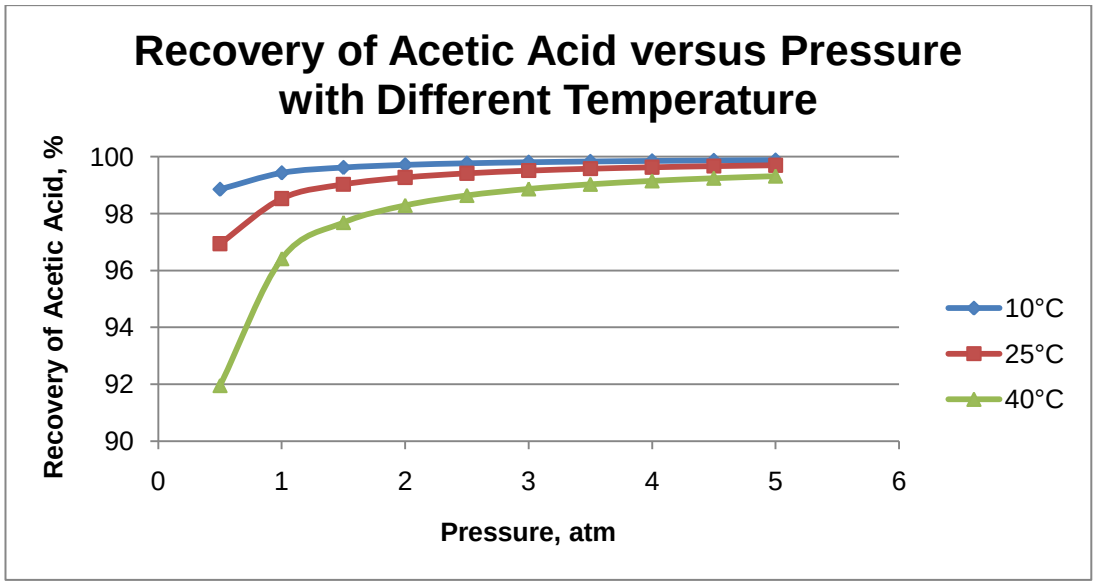


Figure 4.5 Recovery of Acetic Acid versus Pressure with Different Temperature at Flash Drum (T-301)

```
OPTIMIZATION: T301-PRE
----------------------

  SAMPLED VARIABLES:
    ACRY      : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
    ACET      : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
    TACRY     : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
    TACET     : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

  FORTRAN STATEMENTS:
          REACRY=ACRY/TACRY*100
          REACET=ACET/TACET*100

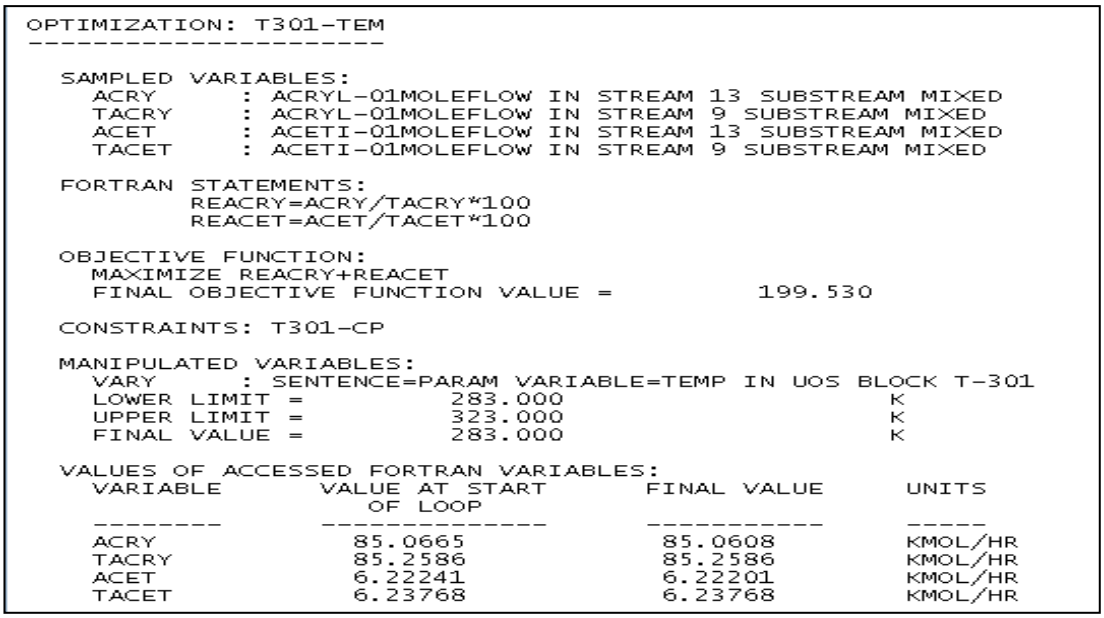
  OBJECTIVE FUNCTION:
    MAXIMIZE REACRY+REACET
    FINAL OBJECTIVE FUNCTION VALUE =          198.505

  CONSTRAINTS: T301-CT

  MANIPULATED VARIABLES:
    VARY      : SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK T-301
    LOWER LIMIT =      101,325.                          N/SQM
    UPPER LIMIT =      506,625.                          N/SQM
    FINAL VALUE =      490,207.                          N/SQM

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE       VALUE AT START       FINAL VALUE      UNITS
                      OF LOOP
    --------       --------------       -----------      -----
    ACRY             83.8644             84.5995        KMOL/HR
    ACET             6.14580             6.19265        KMOL/HR
    TACRY            85.2586             85.2586        KMOL/HR
    TACET            6.23768             6.23768        KMOL/HR
```

Figure 4.6 Optimization Data of Flash Drum with Constant Temperature (T-301)



```
OPTIMIZATION: T301-TEM
----------------------

  SAMPLED VARIABLES:
    ACRY      : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
    TACRY     : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
    ACET      : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
    TACET     : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

  FORTRAN STATEMENTS:
           REACRY=ACRY/TACRY*100
           REACET=ACET/TACET*100

  OBJECTIVE FUNCTION:
    MAXIMIZE REACRY+REACET
    FINAL OBJECTIVE FUNCTION VALUE =          199.530

  CONSTRAINTS: T301-CP

  MANIPULATED VARIABLES:
    VARY      : SENTENCE=PARAM VARIABLE=TEMP IN UOS BLOCK T-301
    LOWER LIMIT =          283.000                      K
    UPPER LIMIT =          323.000                      K
    FINAL VALUE =          283.000                      K

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE       VALUE AT START       FINAL VALUE      UNITS
                      OF LOOP
    --------       --------------       -----------      -----
    ACRY              85.0665             85.0608        KMOL/HR
    TACRY             85.2586             85.2586        KMOL/HR
    ACET              6.22241             6.22201        KMOL/HR
    TACET             6.23768             6.23768        KMOL/HR
```

Figure 4.7 Optimization Data of Flash Drum with Constant Pressure (T-301)

After sensitivity analysis were conducted, the suitable range for pressure is varied from 0.5atm to 5atm and the suitable range of temperature is varied from 10℃ to 40℃. From the Figure 4.4 and 4.5, the recovery of acids depends on the operating pressure and temperature of the flash drum. As the operating pressure increased, recovery of both acids also increased. However, as the temperature increased, the recovery of both acids decreased.

Hence, the optimum condition must be kept in high pressure but low temperature. For the optimum conditions for flash drum, the pressure must be above 1atm in order to obtain more than 99% recovery of acids. From the Figure 4.6 and 4.7, in order to obtain maximum recovery of acrylic acid and acetic acid, optimum pressure and temperature are 490207N/SQM or 4.84atm and 283K or 10℃ respectively. However, temperature at 25℃ is recommended because it is at room temperature which did not require any additional energy. Therefore, optimum pressure and temperature are 4.84atm and 25℃ respectively.

4.3.3 Absorption Tower (T-302)

4.3.3.1 Formulation of Optimization Problem (T-302)

The function of absorption tower is to recover back acrylic acid and acetic acid from the upper outlet stream of flash drum by using water as the solvent. Hence, optimization objective for absorption tower is to maximize the percentage recovery of acrylic acid and acetic acid with a minimum molar flow rate of water. Therefore, molar flow rate of water as the manipulated variable while recovery of acrylic acid and acetic acid as the measured variables. The constant variables present are pressure, temperature, and the number of trays in absorption tower.

4.3.3.2 Result and Discussion (T-302)

The result of sensitivity analysis for absorption tower is shown in Table 4.4. Figure 4.8 shows the graph of recovery of acrylic acid and acetic acid versus molar flow rate of water. Besides that, Figure 4.9 shows the optimization data of absorption tower.

Table 4.4 Sensitivity Analysis Data of Absorption Tower (T-302)

Mole Flow Rate of Water, kmol/hr	Recovery of Acrylic Acid	Recovery of Acetic Acid
20	61.33859	71.30993
30	79.70255	91.65829
40	89.27758	97.09286
50	94.17557	98.73016
60	96.70046	99.34117
70	98.03455	99.61382
80	98.75695	99.75049
90	99.16839	99.8265
100	99.41531	99.87233
110	99.57098	99.90178
120	99.67359	99.92172
130	99.74392	99.9358
140	99.79381	99.94611
150	99.82992	99.95381

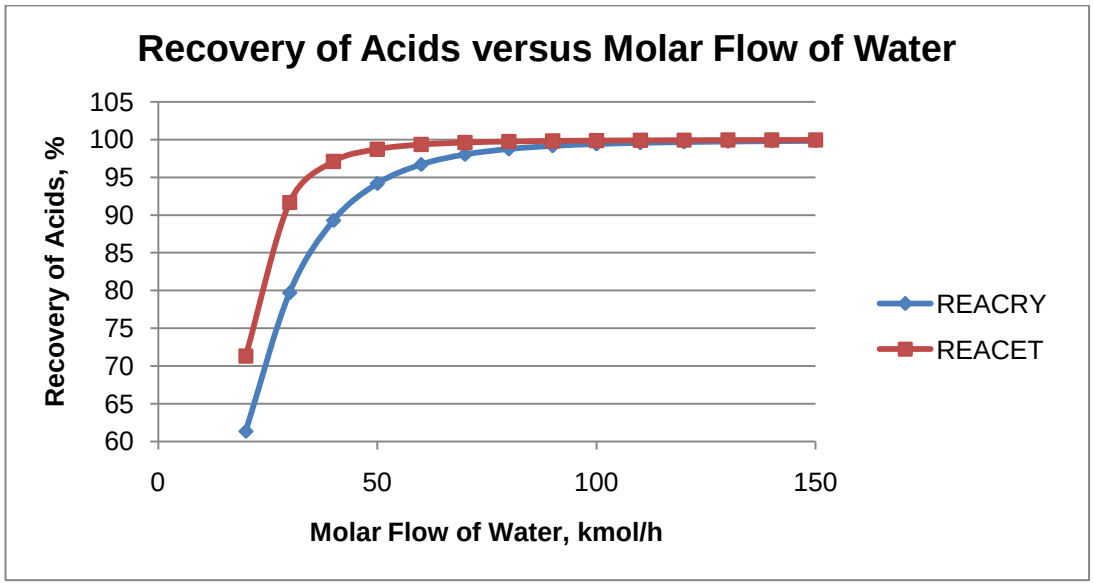
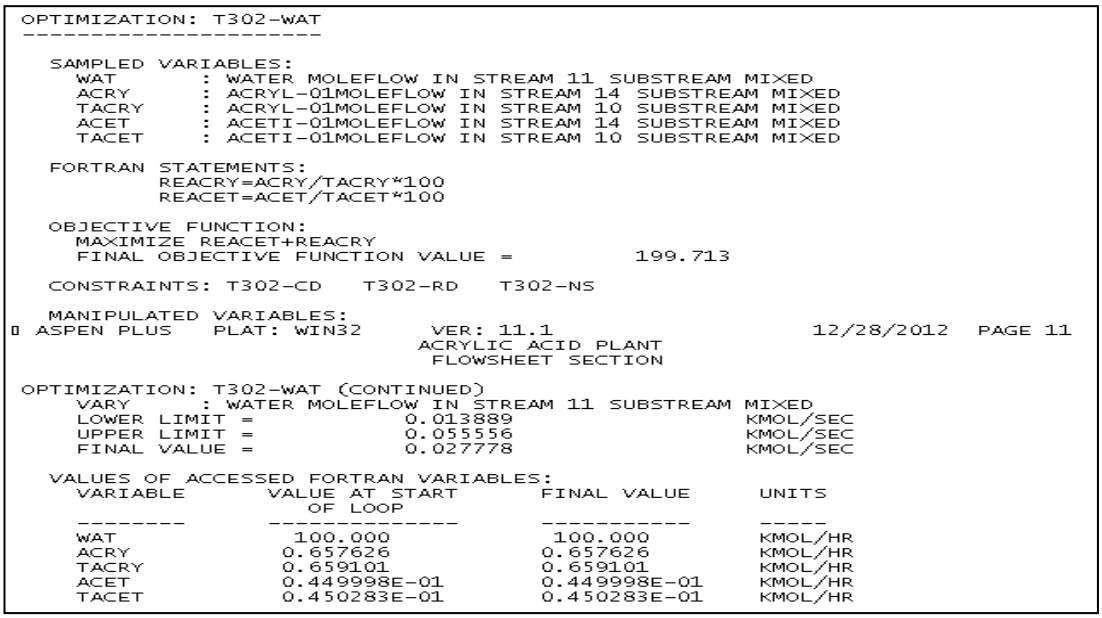


Figure 4.8 Recovery of Acids versus Molar Flow of Water of Absorption Tower (T-302)



```
 OPTIMIZATION: T302-WAT
 ----------------------

   SAMPLED VARIABLES:
     WAT       : WATER MOLEFLOW IN STREAM 11 SUBSTREAM MIXED
     ACRY      : ACRYL-01MOLEFLOW IN STREAM 14 SUBSTREAM MIXED
     TACRY     : ACRYL-01MOLEFLOW IN STREAM 10 SUBSTREAM MIXED
     ACET      : ACETI-01MOLEFLOW IN STREAM 14 SUBSTREAM MIXED
     TACET     : ACETI-01MOLEFLOW IN STREAM 10 SUBSTREAM MIXED

   FORTRAN STATEMENTS:
            REACRY=ACRY/TACRY*100
            REACET=ACET/TACET*100

   OBJECTIVE FUNCTION:
     MAXIMIZE REACET+REACRY
     FINAL OBJECTIVE FUNCTION VALUE =          199.713

   CONSTRAINTS: T302-CD   T302-RD   T302-NS

   MANIPULATED VARIABLES:
 ASPEN PLUS   PLAT: WIN32      VER: 11.1                      12/28/2012  PAGE 11
                              ACRYLIC ACID PLANT
                               FLOWSHEET SECTION

 OPTIMIZATION: T302-WAT (CONTINUED)
     VARY      : WATER MOLEFLOW IN STREAM 11 SUBSTREAM MIXED
     LOWER LIMIT =            0.013889                    KMOL/SEC
     UPPER LIMIT =            0.055556                    KMOL/SEC
     FINAL VALUE =            0.027778                    KMOL/SEC

   VALUES OF ACCESSED FORTRAN VARIABLES:
     VARIABLE       VALUE AT START       FINAL VALUE      UNITS
                      OF LOOP
     --------       --------------       -----------      -----
     WAT              100.000             100.000         KMOL/HR
     ACRY            0.657626            0.657626         KMOL/HR
     TACRY           0.659101            0.659101         KMOL/HR
     ACET          0.449998E-01        0.449998E-01       KMOL/HR
     TACET         0.450283E-01        0.450283E-01       KMOL/HR
```

Figure 4.9 Optimization Data of Absorption Tower (T-302)

After sensitivity analysis, the suitable range of water flow rate is from 20 kmol/h to 150 kmol/h. From Figure 4.8, the recovery of acrylic acid and acetic acid depends on the molar flow rate of water. As the molar flow rate of water increased, the recovery of the acids also increased. However, recovery of acrylic acid required more flow rate of water to separate it out from the mixture. Since acrylic acid is the desired product, hence the optimum condition is based on the recovery of acrylic acid. Therefore, the recommend optimum molar water flow rate must be above 90 kmol/h. From the Figure 4.9, it shows that in order to maximize the recovery of acrylic acid and acetic acid, optimum molar flow rate of water is 0.027778 kmol/sec or 100kmol/h.

4.3.4 Liquid-liquid Extractor (T-303)

4.3.4.1 Formulation of Optimization Problem (T-303)

The function of liquid-liquid extractor is to separate out the acrylic acid and acetic acid from the water by using diisopropyl ether (DIPE) as the solvent. The optimization objective is to maximize the recovery of acrylic acid and acetic acid with a minimum molar flow rate of solvent. Hence, molar flow rate of solvent as the manipulated variable and recovery of acrylic acid and acetic acid as the measured variables. The constant variables are pressure, temperature, the number of trays and feed location into absorption tower.

4.3.4.2 Result and Discussion (T-303)

The result of sensitivity analysis of liquid-liquid extractor is shown in Table 4.5. The Figure 4.10 shows the graph of recovery of acrylic acid and acetic acid versus molar flow rate of water. Besides that, Figure 4.11 shows the optimization data of liquid-liquid extractor.

Table 4.5 Sensitivity Analysis Data of Liquid-liquid Extractor (T-303)

Mole Flow Rate of DIISO, kmol/h	Recovery of Acrylic Acid	Recovery of Acetic Acid
50	54.33891	17.99589
150	98.44178	37.08619
250	99.96867	44.80824
350	99.99943	52.32332
450	99.99998	59.99881
550	100	67.79101
650	100	75.6926
750	100	83.34827
850	100	90.02937
950	100	94.89823
1050	100	97.71632
1150	100	99.05802
1250	100	99.62319
1350	100	99.84587

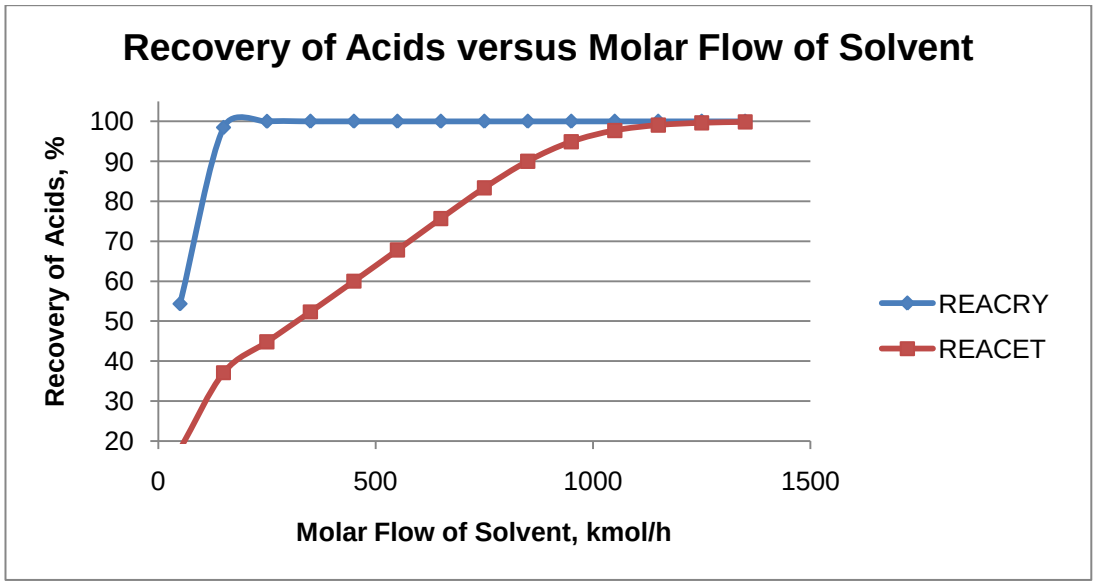
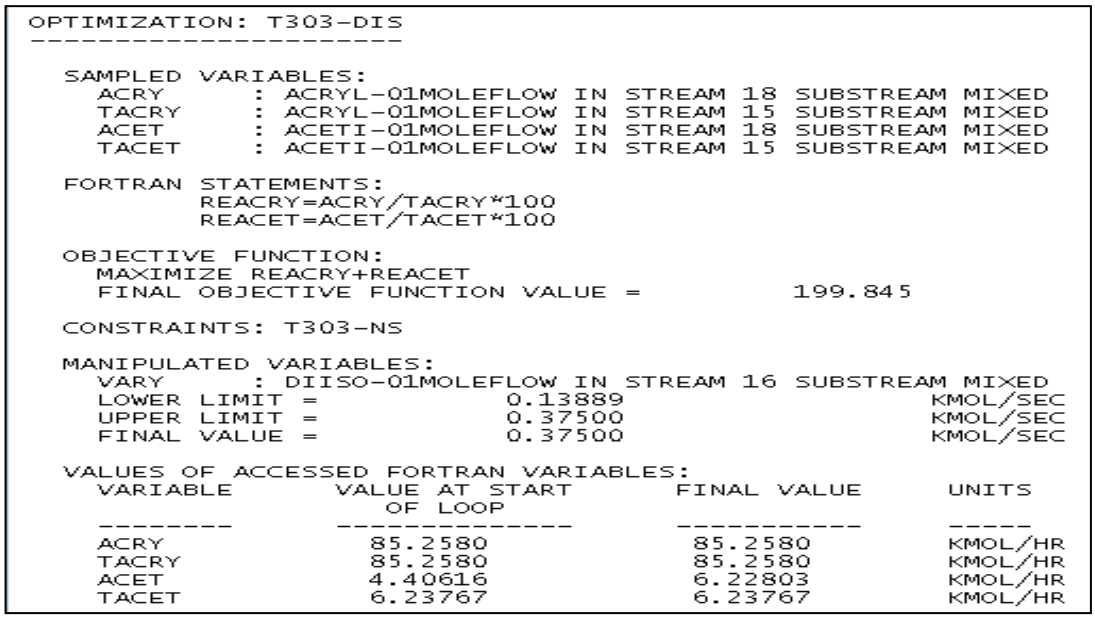


Figure 4.10 Recovery of Acids versus Molar Flow Rate of Solvent of Liquid-liquid Extractor (T-303)



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OPTIMIZATION: T303-DIS
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  SAMPLED VARIABLES:
    ACRY      : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
    TACRY     : ACRYL-01MOLEFLOW IN STREAM 15 SUBSTREAM MIXED
    ACET      : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
    TACET     : ACETI-01MOLEFLOW IN STREAM 15 SUBSTREAM MIXED

  FORTRAN STATEMENTS:
            REACRY=ACRY/TACRY*100
            REACET=ACET/TACET*100

  OBJECTIVE FUNCTION:
    MAXIMIZE REACRY+REACET
    FINAL OBJECTIVE FUNCTION VALUE =          199.845

  CONSTRAINTS: T303-NS

  MANIPULATED VARIABLES:
    VARY      : DIISO-01MOLEFLOW IN STREAM 16 SUBSTREAM MIXED
    LOWER LIMIT =             0.13889                    KMOL/SEC
    UPPER LIMIT =             0.37500                    KMOL/SEC
    FINAL VALUE =             0.37500                    KMOL/SEC

  VALUES OF ACCESSED FORTRAN VARIABLES:
    VARIABLE       VALUE AT START       FINAL VALUE      UNITS
                      OF LOOP
    --------       --------------       -----------      -----
    ACRY              85.2580              85.2580        KMOL/HR
    TACRY             85.2580              85.2580        KMOL/HR
    ACET              4.40616              6.22803        KMOL/HR
    TACET             6.23767              6.23767        KMOL/HR
```

Figure 4.11 Optimization Data of Liquid-liquid Extractor (T-303)

After analysis by sensitivity method, the range of manipulated variable or molar flow rate of solvent is from 50 kmol/h to 1350 kmol/h. From Figure 4.10, the recovery of acrylic acid and acetic acid depends on the molar flow rate of solvent. As the molar flow of solvent increased, the recovery of acids also increased. However, the recovery percentage for both acids is different. For the acrylic acid, minimum molar flow rate of solvent required is around 250 kmol/h. However, for the acetic acid is around 1250 kmol/h. Therefore, the recommend optimum solvent molar flow rate must be more than 1250 kmol/h in order to achieve more than 99% recovery of acetic acid. From the Figure 4.11, in order to obtain maximum recovery of acrylic acid and acetic acid, the molar flow rate of solvent is 0.37500kmol/sec or 1350kmol/h.

4.3.5 Distillation Column 1 (T-304)

4.3.5.1 Formulation of Optimization Problem (T-304)

The function of the distillation column 1 is to separate out the solvent or diisopropyl ether from the acids mixture. At distillation column, solvent is retrieved at the top while acids are presents at the bottom stream. The optimization objectives of the first distillation column are to maximize separation efficiency of solvent and maximized recovery percentage of acrylic acid and acetic acid. During optimization, the pressure and distillate rate is kept constant at 0.1atm and 1362.58kmol/h respectively. The optimization parameters are feed stages location, reflux ratio, and re-boiler heat duty.

4.3.5.2 Feed Stages Location Optimization (T-304)

For feed stages location optimization, the manipulated variable present is the location of the feed stages while number of stages, reflux ratio, and distillate rate are the constant variables. The number of stages and reflux ratio are kept fixed at 15 stages and 3 respectively. The feed trays location is varied from trays number 1 to number 15. The result of sensitivity analysis of feed stages location of distillation column 1 is shown in Table 4.6. The Figure 4.12 shows the graph of recovery of acrylic acid, acetic acid and solvent versus feed stages location of the distillation column 1.

Table 4.6 Sensitivity Analysis Data of Feed Stages Location of Distillation Column 1 (T-304)

Feed Stages	Recovery of Acrylic Acid	Recovery of Acetic Acid	Recovery of Diisopropyl Ether
1	73.11562	70.11368	97.92958
2	96.94891	92.19902	99.6658
3	99.41613	96.87779	99.85758
4	99.88053	98.6732	99.89828
5	99.97533	99.42949	99.90856
6	99.99489	99.75332	99.91152
7	99.99894	99.89281	99.9125
8	99.99978	99.95253	99.91286
9	99.99995	99.97796	99.913
10	99.99999	99.98854	99.91307
11	100	99.99252	99.91319
12	100	99.99347	99.91374
13	100	99.99293	99.91695
14	100	99.99131	99.93712
15	100	99.9844	99.95369

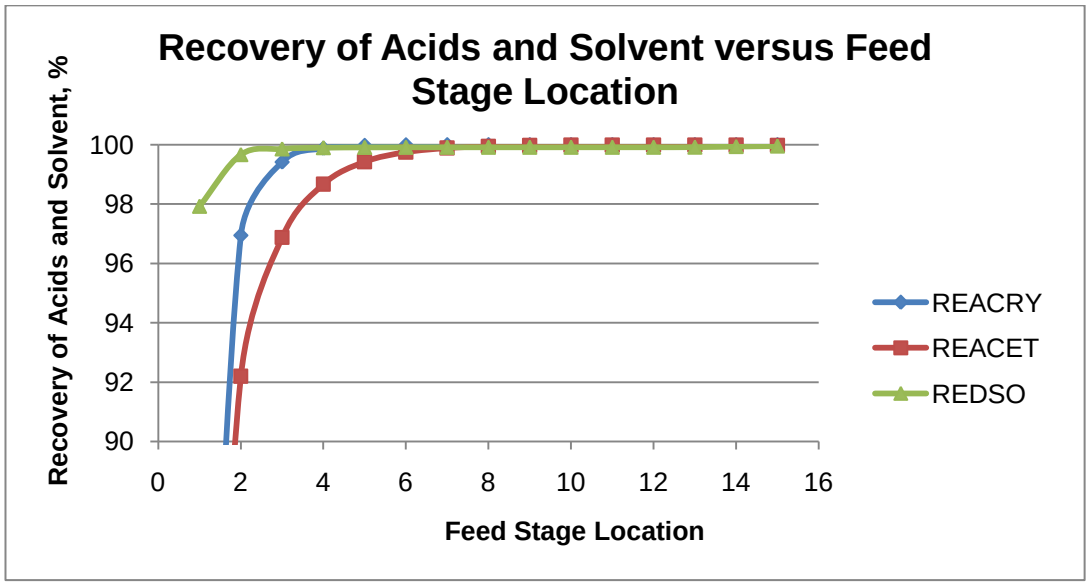


Figure 4.12 Recovery of Acids and Solvent versus Feed Stage Location of Distillation Column 1 (T-304)

From Figure 4.12, the recovery of acrylic acid, acetic acid and solvent depends on the feed stages location. As the feed stage location located at a higher

position, the percentage of recovery also increased but the saturated point is reached when feed stages location is almost at the 8th stage. Therefore, for the optimum condition, the location at the feed stage is at the 8th stage so as to obtain more than 99.9% of recovery.

4.3.5.3 Reflux Ratio Optimization (T-304)

For the reflux ratio optimization, reflux ratio is the manipulated variable but number of stages, feed stages location and distillate rate are constant variables. The number of stages and feed stages location are kept fixed at 15 stages and at the 8th stage respectively. After sensitivity analysis was carried out, the range of reflux ratio to be manipulated is varied from 0.5 to 10. The result of sensitivity analysis of reflux ratio of distillation column 1 is shown in Table 4.7. Figure 4.13 shows the graph of percentage recovery of acrylic acid, acetic acid and solvent versus reflux ratio of distillation column 1. Besides that, Figure 4.14 shows the optimization data of distillation column 1 with reflux ratio as optimization parameter.

Table 4.7 Sensitivity Analysis Data of Reflux Ratio of Distillation Column 1 (T-304)

Reflux Ratio	Recovery of Acrylic Acid	Recovery of Acetic Acid	Recovery of Diisopropyl Ether
0.5	99.27205	93.71747	99.831841
1	99.64451	96.45311	99.871012
1.5	99.7636	97.51386	99.884473
2	99.8222	98.07899	99.891314
2.5	99.8572	98.43156	99.895476
3	99.88054	98.67323	99.898284
3.5	99.89724	98.84955	99.900311
4	99.9098	98.98402	99.901844
4.5	99.91958	99.09001	99.903045
5	99.92745	99.17594	99.904015
5.5	99.93391	99.24683	99.904812
6	99.9393	99.30639	99.905479
6.5	99.94387	99.35716	99.906047
7	99.9478	99.40096	99.906535
7.5	99.95121	99.43914	99.90696
8	99.9542	99.47272	99.907333
8.5	99.95685	99.50248	99.907663
9	99.9592	99.52904	99.907957
9.5	99.96131	99.5529	99.908221
10	99.96321	99.57444	99.90846

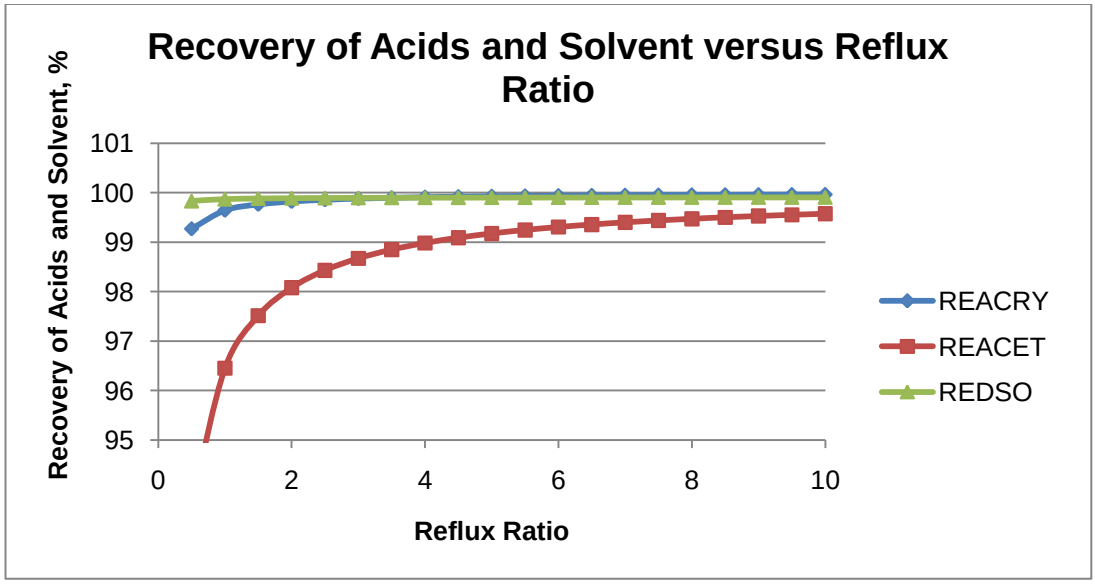
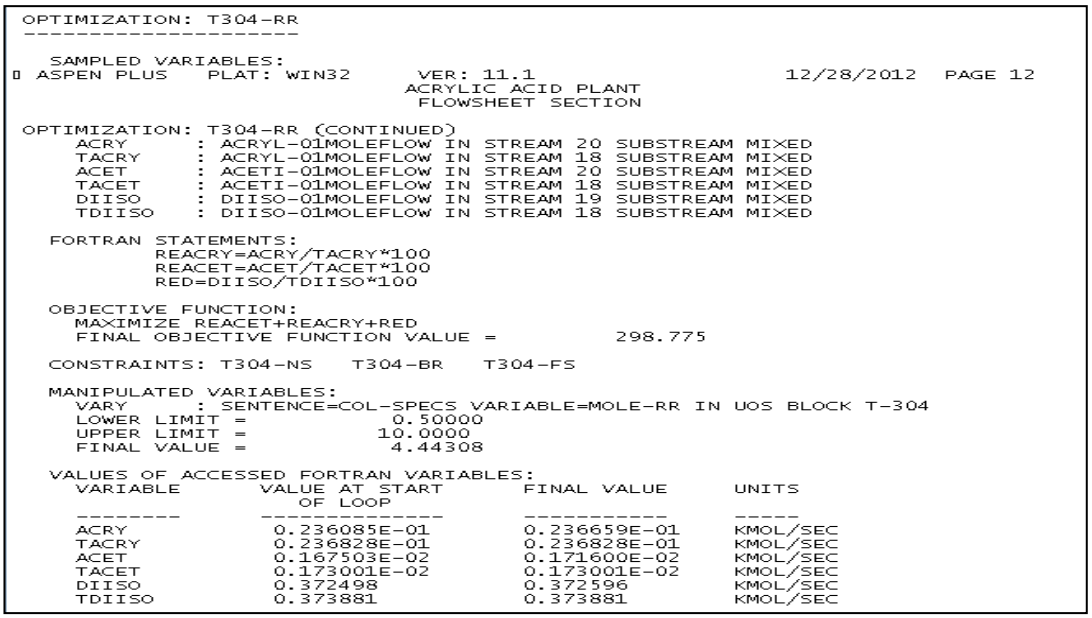


Figure 4.13 Recovery of Acids and Solvent versus Reflux Ratio of Distillation Column 1 (T-304)



```
 OPTIMIZATION: T304-RR
 ---------------------

   SAMPLED VARIABLES:
 ASPEN PLUS   PLAT: WIN32      VER: 11.1                      12/28/2012  PAGE 12
                              ACRYLIC ACID PLANT
                               FLOWSHEET SECTION

 OPTIMIZATION: T304-RR (CONTINUED)
     ACRY      : ACRYL-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
     TACRY     : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
     ACET      : ACETI-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
     TACET     : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
     DIISO     : DIISO-01MOLEFLOW IN STREAM 19 SUBSTREAM MIXED
     TDIISO    : DIISO-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED

   FORTRAN STATEMENTS:
           REACRY=ACRY/TACRY*100
           REACET=ACET/TACET*100
           RED=DIISO/TDIISO*100

   OBJECTIVE FUNCTION:
     MAXIMIZE REACET+REACRY+RED
     FINAL OBJECTIVE FUNCTION VALUE =          298.775

   CONSTRAINTS: T304-NS   T304-BR   T304-FS

   MANIPULATED VARIABLES:
     VARY      : SENTENCE=COL-SPECS VARIABLE=MOLE-RR IN UOS BLOCK T-304
     LOWER LIMIT =            0.50000
     UPPER LIMIT =           10.0000
     FINAL VALUE =            4.44308

   VALUES OF ACCESSED FORTRAN VARIABLES:
     VARIABLE       VALUE AT START       FINAL VALUE      UNITS
                       OF LOOP
     --------       --------------       -----------      -----
     ACRY            0.236085E-01        0.236659E-01     KMOL/SEC
     TACRY           0.236828E-01        0.236828E-01     KMOL/SEC
     ACET            0.167503E-02        0.171600E-02     KMOL/SEC
     TACET           0.173001E-02        0.173001E-02     KMOL/SEC
     DIISO           0.372498            0.372596         KMOL/SEC
     TDIISO          0.373881            0.373881         KMOL/SEC
```

Figure 4.14 Optimization Data of Distillation Column 1 with Reflux Ratio Optimization Parameter (T-304)

From the Figure 4.13, the recovery of acrylic acid, acetic acid and solvent depends on reflux ratio. As the reflux ratio increased, the recovery of acids and solvent also increased. For the optimum condition, reflux ratio must be more than 5 in order to get more than 99% recovery of acids and solvent. However, From the Figure 4.14, in order to get maximum recovery of acids and solvent, optimum reflux ratio is 4.44308.

4.3.5.4 Re-boiler Heat Duty Optimization (T-304)

For the re-boiler heat duty optimization, re-boiler heat duty is the manipulated variable but number of stages, feed stages location, distillate rate, and reflux ratio are constant variables. The number of stages, reflux ratio and feed stages location are kept fixed at 15 stages, reflux ratio of 3 and the feed location is at the 8th

stage respectively. After sensitivity analysis, the suitable range of re-boiler heat duty is varied from 40000MJ/h to 300000MJ/h. The result of sensitivity analysis of re-boiler heat duty of distillation column 1 is shown in Table 4.8. Figure 4.15 shows the graph of recovery of acrylic acid, acetic acid and solvent versus re-boiler heat duty of distillation column 1. Moreover, Figure 4.16 shows the optimization data of distillation column 1 with re-boiler heat duty as optimization parameter.

Table 4.8 Sensitivity Analysis Data of Re-boiler Heat Duty for Distillation Column 1 (T-304)

Re-boiler Duty, MJ/h	Recovery of Acrylic Acid	Recovery of Acetic Acid	Recovery of Diisopropyl Ether
40000	91.08283	76.991117	99.18925
60000	98.73016	90.761728	99.78001
80000	99.37097	94.372839	99.84189
100000	99.5843	95.956771	99.86441
120000	99.6889	96.835863	99.87597
140000	99.75092	97.395637	99.88301
160000	99.79199	97.783918	99.88777
180000	99.82124	98.069524	99.8912
200000	99.84316	98.288688	99.8938
220000	99.8602	98.46238	99.89584
240000	99.87386	98.60354	99.89748
260000	99.88505	98.720602	99.89883
280000	99.89439	98.8193	99.89996
300000	99.90231	98.903677	99.90093

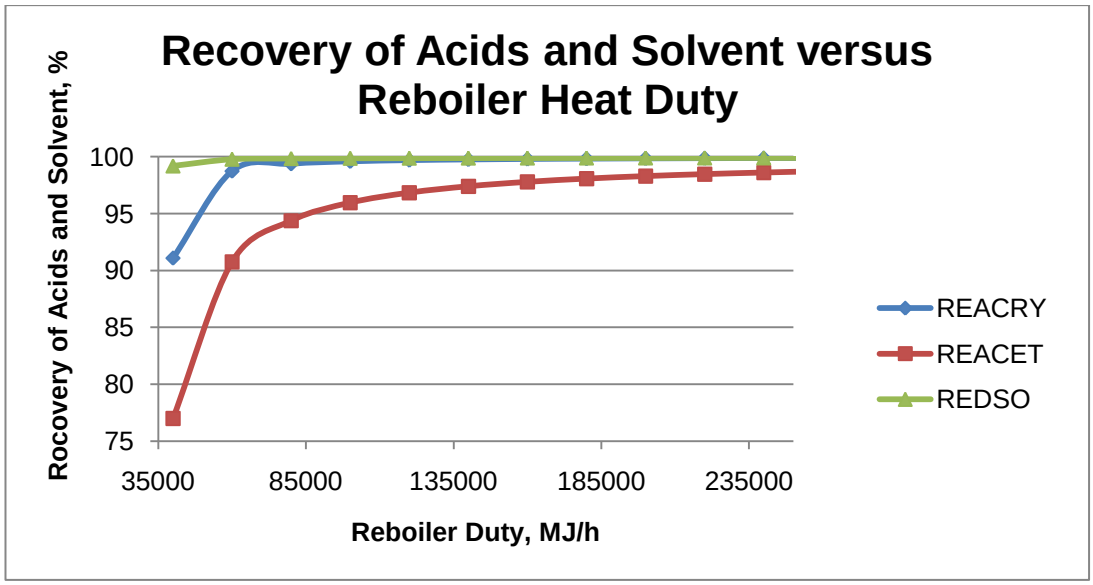


Figure 4.15 Recovery of Acids and Solvent versus Re-boiler Heat Duty of Distillation Column 1 (T-304)

```
 OPTIMIZATION: T304-RD
 ---------------------

   SAMPLED VARIABLES:
 ASPEN PLUS    PLAT: WIN32      VER: 11.1                        12/28/2012   PAGE 12
                               ACRYLIC ACID PLANT
                                FLOWSHEET SECTION

 OPTIMIZATION: T304-RD (CONTINUED)
      ACRY      : ACRYL-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
      TACRY     : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
      ACET      : ACETI-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
      TACET     : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
      DIISO     : DIISO-01MOLEFLOW IN STREAM 19 SUBSTREAM MIXED
      TDIISO    : DIISO-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED

    FORTRAN STATEMENTS:
             REACRY=ACRY/TACRY*100
             REACET=ACET/TACET*100
             RED=DIISO/TDIISO*100

    OBJECTIVE FUNCTION:
      MAXIMIZE REACET+REACRY+RED
      FINAL OBJECTIVE FUNCTION VALUE =          298.407

    CONSTRAINTS: T304-NS    T304-BR    T304-FS

    MANIPULATED VARIABLES:
      VARY      : SENTENCE=COL-SPECS VARIABLE=QN IN UOS BLOCK T-304
      LOWER LIMIT =    9,722,230.                        WATT
      UPPER LIMIT =            0.833333+08               WATT
      FINAL VALUE =            0.833333+08               WATT

    VALUES OF ACCESSED FORTRAN VARIABLES:
      VARIABLE        VALUE AT START        FINAL VALUE      UNITS
                        OF LOOP
      --------      ---------------       -----------      -----
      ACRY           0.235761E-01         0.236585E-01     KMOL/SEC
      TACRY          0.236828E-01         0.236828E-01     KMOL/SEC
      ACET           0.165544E-02         0.171023E-02     KMOL/SEC
      TACET          0.173001E-02         0.173001E-02     KMOL/SEC
      DIISO          0.372446             0.372583         KMOL/SEC
      TDIISO         0.373881             0.373881         KMOL/SEC
```

Figure 4.16 Optimization Data of Distillation Column 1 with Re-boiler Heat Duty Optimization Parameter (T-304)

From the Figure 4.15, the recovery of acrylic acid, acetic acid and solvent are depends on the re-boiler heat duty supply. As the re-boiler heat duty is increased, the recovery of acids and solvent also increased. For the optimum re-boiler heat duty, it

must be supply around 200000MJ/h to the distillation column to achieve at least 99% of recovery. From the Figure 4.16, in order to maximize recovery of acids and solvent, optimum re-boiler heat duty is 0.833333E8 watt or 300000MJ/h. However, as more re-boiler heat duty supply, more operating cost required. In order to save operation cost, 180000MJ/h is recommended.

4.3.6 Distillation Column 2 (T-305)

4.3.6.1 Formulation of Optimization Problem (T-305)

The function of distillation column 2 is to separate out the desired product (acrylic acid) and the by product (acetic acid). Since acetic acid has lower boiling point than acrylic acid, hence top product is acetic acid whereas the bottom product is acrylic acid. The optimization objective for distillation column 2 is to maximize the purity of both acrylic acid and acetic acid by varying the optimization parameters which are feed stages location, reflux ratio and re-boiler heat duty. During the optimization, constant variables present are pressure, distillate rate and number of stage which kept constant at 0.1atm, 8kmol/h and 36 stages respectively.

4.3.6.2 Feed Stages Location Optimization (T-305)

For feed stages location optimization, feed stages location is the manipulated variable but the number of stages, reflux ratio, and distillate rate are constant

variables. The number of stages and reflux ratio are kept fixed at 36 stages and 12 respectively. The feed stages location is varied from stage number 2 to 36 in order to observe all variation of purity of acids. The result of sensitivity analysis of feed stages location for distillation column 2 is shown in Table 4.9. The Figure 4.17 shows the graph of recovery of acrylic acid and acetic acid versus feed stage location of distillation column 2.

Table 4.9 Sensitivity Analysis Data of Feed Stages Location of Distillation Column 2 (T-305)

Feed Stages Location	Purity of Acrylic Acid	Purity of Acetic Acid	Feed Stages Location	Purity of Acrylic Acid	Purity of Acetic Acid
2	97.2164389	48.05287	20	99.9883407	78.54379
3	98.5367982	62.57683	21	99.9838279	78.49415
4	99.3338823	71.34475	22	99.9775811	78.42544
5	99.7446985	75.86373	23	99.9689456	78.33045
6	99.9252014	77.84926	24	99.9570122	78.19918
7	99.9910821	78.57395	25	99.9405463	78.01806
8	99.9984437	78.65493	26	99.9178473	77.76837
9	99.9991439	78.66263	27	99.8865746	77.42437
10	99.9992927	78.66427	28	99.8434897	76.95043
11	99.9992495	78.66379	29	99.7840539	76.29664
12	99.9990793	78.66192	30	99.7018042	75.3919
13	99.9987864	78.6587	31	99.5873644	74.13314
14	99.9983507	78.6539	32	99.4263772	72.36277
15	99.9977287	78.64706	33	99.1958706	69.83065
16	99.9968557	78.63746	34	98.8556865	66.11265
17	99.9956386	78.62407	35	98.3230014	60.42069
18	99.9939464	78.60546	36	97.3695729	51.10874
19	99.9915977	78.57962			

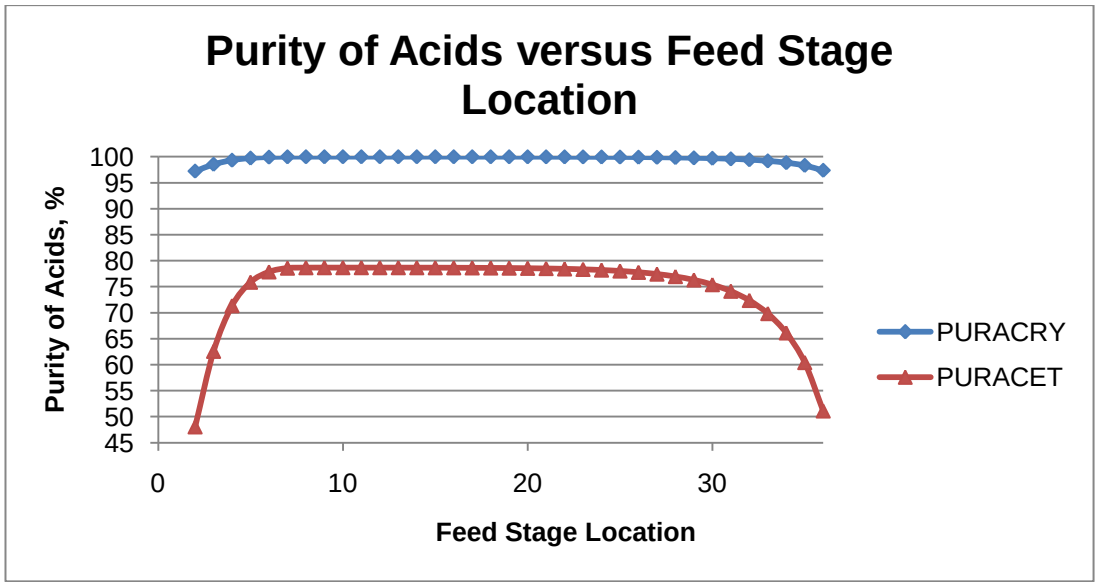


Figure 4.17 Recovery of Acids versus Feed Stage Location of Distillation Column 2 (T-305)

From the Figure 4.17, the purity of acrylic acid and acetic acid depends on feed stages location. For the optimum feed stages location, feed stage must be between stages of 8^{th} to 25^{th} in order to obtain maximum purity of acids. Hence, according to the reference of previous chapter, 23^{th} feed stage location is chosen as the optimum stage for distillation column 2.

4.3.6.3 Reflux Ratio Optimization (T-305)

For the reflux ratio optimization, reflux ratio is the manipulated variable but number of stages, feed stages location and distillate rate are constant variables. The number of stages and feed stages location are kept fixed at 36 stages and 23th stage respectively. After sensitivity analysis, the suitable range of reflux ratio to be manipulated is varied from 1 to 15. The result of sensitivity analysis of reflux ratio for distillation column 2 is shown in Table 4.10. Figure 4.18 shows the graph of

recovery of acrylic acid and acetic acid versus the reflux ratio of distillation column 2. Besides that, Figure 4.19 shows the optimization data of distillation column 2 with reflux ratio as the optimization parameter.

Table 4.10 Sensitivity Analysis Data of Reflux Ratio for Distillation Column 2 (T-305)

Reflux Ratio, RR	Purity of Acrylic Acid	Purity of Acetic Acid
1	95.02708	23.96998
2	95.95845	34.21501
3	96.84466	43.96334
4	97.67569	53.10468
5	98.42036	61.296
6	99.0279	67.97892
7	99.45494	72.67644
8	99.70905	75.47159
9	99.84396	76.95562
10	99.91327	77.71807
11	99.94934	78.1148
12	99.96897	78.33068
13	99.98014	78.45359
14	99.98679	78.5267
15	99.9909	78.57196

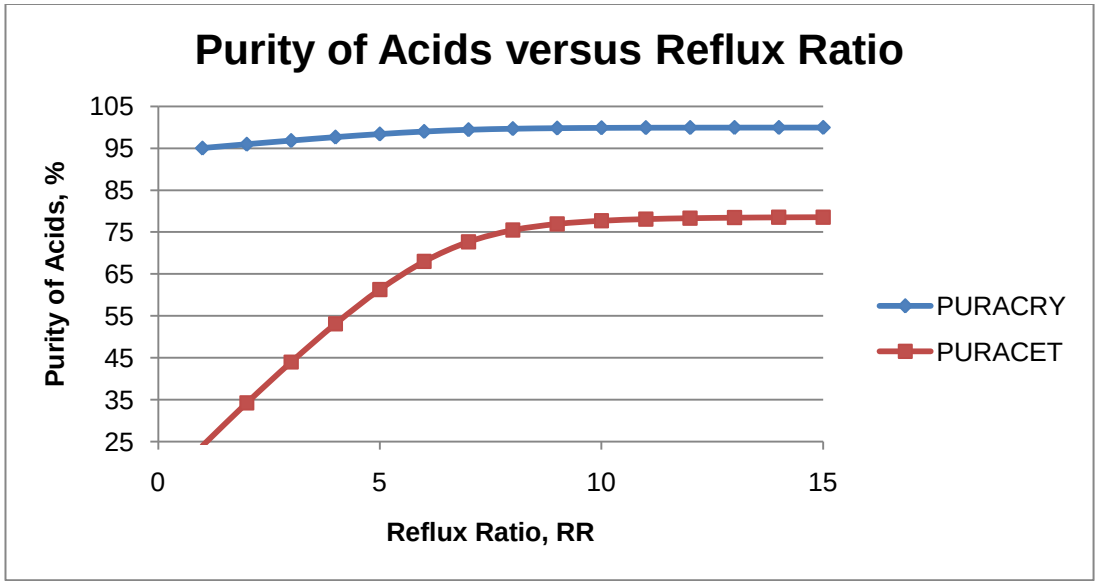


Figure 4.18 Recovery of Acids and Solvent versus Reflux Ratio of Distillation Column 2 (T-305)

```
 OPTIMIZATION: T305-RR
 ---------------------

   SAMPLED VARIABLES:
     ACRY      : ACRYL-01MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
     TOTAL1    : TOTAL MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
     ACET      : ACETI-01MOLEFLOW IN STREAM 21 SUBSTREAM MIXED
     TOTAL2    : TOTAL MOLEFLOW IN STREAM 21 SUBSTREAM MIXED

   FORTRAN STATEMENTS:
          PUR1=ACRY/TOTAL1*100
          PUR2=ACET/TOTAL2*100

   OBJECTIVE FUNCTION:
     MAXIMIZE PUR1+PUR2
     FINAL OBJECTIVE FUNCTION VALUE =          177.842

   CONSTRAINTS: T305-BR    T305-FS    T305-NS
 ASPEN PLUS    PLAT: WIN32      VER: 11.1                    12/28/2012  PAGE 13
                              ACRYLIC ACID PLANT
                               FLOWSHEET SECTION

 OPTIMIZATION: T305-RR (CONTINUED)

   MANIPULATED VARIABLES:
     VARY      : SENTENCE=COL-SPECS VARIABLE=MOLE-RR IN UOS BLOCK T-305
     LOWER LIMIT =           10.0000
     UPPER LIMIT =           15.0000
     FINAL VALUE =           10.5000

   VALUES OF ACCESSED FORTRAN VARIABLES:
     VARIABLE       VALUE AT START      FINAL VALUE      UNITS
                        OF LOOP
     --------       --------------      -----------      -----
     ACRY            0.236659E-01       0.236659E-01     KMOL/SEC
     TOTAL1          0.250000E-01       0.250000E-01     KMOL/SEC
     ACET            0.381857E-03       0.381857E-03     KMOL/SEC
     TOTAL2          0.166667E-02       0.166667E-02     KMOL/SEC
```

Figure 4.19 Optimization Data of Distillation Column 2 with Reflux Ratio Optimization Parameter (T-305)

From Figure 4.18, the purity of acrylic acid and acetic acid depends on reflux ratio. As the reflux ratio is increased, the purity of acids is also increased. For the optimum reflux ratio, it must be above 9 in order to achieve maximum purity of acids respectively. From Figure 4.19, it shows that the optimum reflux ratio of distillation column 2 is 10.5.

4.3.6.4 Re-boiler Heat Duty Optimization (T-305)

For the re-boiler heat duty optimization, re-boiler heat duty is the manipulated variable but number of stages, feed stages location, distillate rate, and reflux ratio are constant variables. The number of stages, reflux ratio and feed stages location are kept fixed at 15 stages, 3 and the 8^{th} stage respectively. After sensitivity analysis, the suitable range of re-boiler heat duty is varied from 40000 MJ/h to 300000MJ/h. The result of sensitivity analysis of re-boiler heat duty of distillation

column 2 is shown in Table 4.11. Figure 4.20 shows that the graph of purity of acrylic acid and acetic acid versus re-boiler heat duty of distillation column 2. Besides that, Figure 4.21 shows the optimization data of distillation column 2 with re-boiler heat duty as the optimization parameter.

Table 4.11 Sensitivity Analysis Data of Re-boiler Heat Duty for Distillation Column 2 (T-305)

Re-boiler Duty, MJ/h	Purity of Acrylic Acid, %	Purity of Acetic Acid, %
200	93.9580	14.1543
400	94.3240	18.0517
600	95.1382	27.0038
800	95.9523	35.9584
1000	96.7641	44.8884
1200	97.5634	53.6804
1400	98.3175	61.9762
1600	98.9601	69.0442
1800	99.4192	74.0950
2000	99.6899	77.0728
2200	99.8321	78.6371
2400	99.9055	79.4438
2600	99.9439	79.8662
2800	99.9651	80.0996
3000	99.9774	80.2345

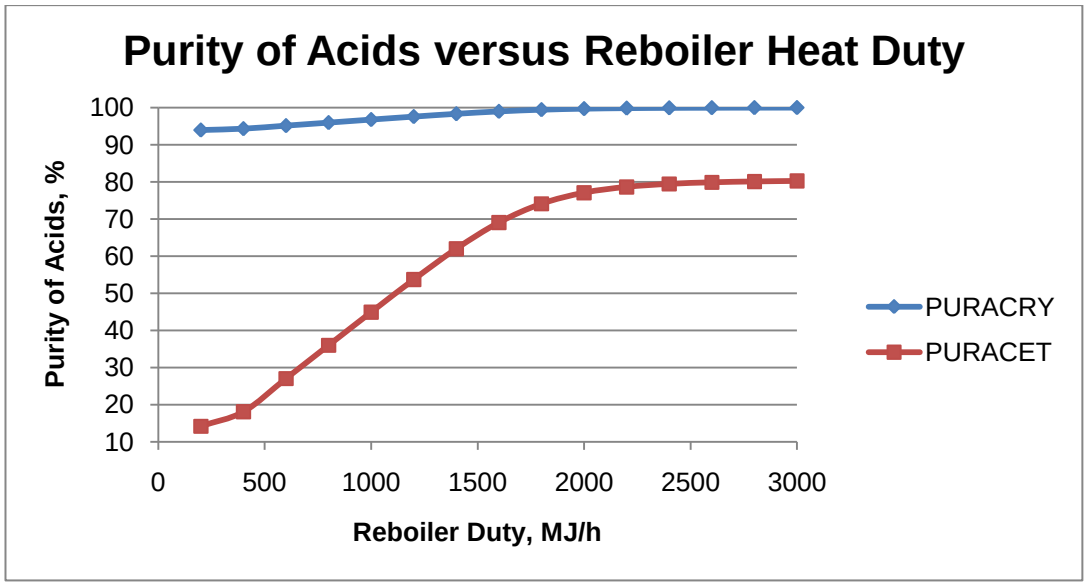


Figure 4.20 Purity of Acids versus Re-boiler Heat Duty of Distillation Column 2 (T-305)

```
 OPTIMIZATION: T305-RD
 ---------------------

    SAMPLED VARIABLES:
      ACRY      : ACRYL-01MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
      TOTAL1    : TOTAL MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
      ACET      : ACETI-01MOLEFLOW IN STREAM 21 SUBSTREAM MIXED
      TOTAL2    : TOTAL MOLEFLOW IN STREAM 21 SUBSTREAM MIXED

    FORTRAN STATEMENTS:
            PUR1=ACRY/TOTAL1*100
            PUR2=ACET/TOTAL2*100

    OBJECTIVE FUNCTION:
      MAXIMIZE PUR1+PUR2
      FINAL OBJECTIVE FUNCTION VALUE =          180.212

    CONSTRAINTS: T305-BR    T305-FS    T305-NS
 ASPEN PLUS    PLAT: WIN32      VER: 11.1                    12/28/2012   PAGE 13
                                ACRYLIC ACID PLANT
                                 FLOWSHEET SECTION

 OPTIMIZATION: T305-RD (CONTINUED)

    MANIPULATED VARIABLES:
      VARY      : SENTENCE=COL-SPECS VARIABLE=QN IN UOS BLOCK T-305
      LOWER LIMIT =       55,556.0                        WATT
      UPPER LIMIT =      833,340.                         WATT
      FINAL VALUE =      833,340.                         WATT

    VALUES OF ACCESSED FORTRAN VARIABLES:
      VARIABLE        VALUE AT START       FINAL VALUE      UNITS
                        OF LOOP
      --------        --------------       -----------      -----
      ACRY             0.236659E-01        0.236659E-01     KMOL/SEC
      TOTAL1           0.250000E-01        0.250000E-01     KMOL/SEC
      ACET             0.381857E-03        0.381857E-03     KMOL/SEC
      TOTAL2           0.166667E-02        0.166667E-02     KMOL/SEC
```

Figure 4.21 Optimization Data of Distillation Column 2 with Re-boiler Heat Duty Optimization Parameter (T-305)

From Figure 4.20, it shows that as the re-boiler heat duty increased, the purity of acrylic acid and acetic acid are also increased but reached a saturated point at around 2000MJ/h. For the optimum condition, the re-boiler heat duty must be

greater than 2000MJ/h in order to obtain maximum purity of both acids respectively. From Figure 4.21, the optimum re-boiler heat duty is 833340 watt or 3000MJ/h.

4.4 Summary

This chapter provides an overview of the descriptive optimization analysis which includes all the reactor and separation units that used to produce the acrylic acid. For the best optimum conditions to be carried out, maximum profit with the minimum operating cost is very important. After overall optimization, the optimum conditions for each unit are obtained in order to obtain maximum production of acrylic acid and desired quality of products.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Introduction

In this study, the main objective is to optimize the operating conditions in the reactor and separators sections of acrylic plant. Besides that, this research is also to simulate the production of acrylic acid process. By conducting this study, the results outcomes had been discussed in the previous chapter which involved simulation and optimization of the acrylic acid plant. In this chapter, the whole study was concluded based on the research founding.

5.2 Conclusions

In the simulation section, the production of acrylic acid process was successful simulated by using Aspen Plus. The basic components of acrylic acid plant are reactors and separators sections. According to the Nirlipt (2010), the cost of materials and products are usually much larger than the costs of energy or capital in a typical chemical process. Hence, the process must be designed and optimized well so

as to not waste feed stocks or lose products (Lubyen, 2010). After optimization, optimum conditions of reactor and separators sections are obtained.

The flow sheet and simulation of acrylic acid production process is successful constructed and simulated. The results of simulation are acceptable because the final production rate of acrylic acid and acetic acid is mostly similar with the references values. The reactor section is optimized by an equilibrium based approach. The optimum value of temperature is 315℃ in order to obtain the maximum yield of acrylic acid which is 0.77254. For the flash drum unit, optimum temperature and pressure are obtained at 25℃ and 4.84atm respectively. Although the temperature to obtain maximum recovery of acrylic and acetic acid is 10℃, however, 25℃ is recommended because at room temperature, additional energy is not required.

For the absorption tower and liquid-liquid extractor, optimum molar flow rate of water and solvent are obtained. From the sensitivity analysis, the minimum molar flow rate of water and solvent are 90kmol/h and 250kmol/h respectively. From the optimization process, the optimum values were obtained which are 100kmol/h and 1350kmol/h respectively in order to recover more than 99% of acrylic and acetic acid.

The two distillation columns in acrylic acid plant depend on a large number of variables. Each manipulated variable is optimized by keeping the other variables as constant. After an optimum value of a variable is obtained, the other manipulated variables are optimized by using that data. For the distillation column 1, the optimum feed stages location is at number eight while the reflux ratio is 4.44308. The re-boiler heat duty is optimized to be 180000MJ/h. For the distillation column 2, the optimum

feed stages location is found to be in the range of 8 to 25 while the reflux ratio is 10.5. The re-boiler heat duty is optimized to be 3000MJ/h.

5.3 Recommendations

During conducting sensitivity analysis and optimization, some cases took place which affects and deviates the results of optimization. There are few recommendations being suggested in order to prevent these incidents. Firstly, for the sensitivity analysis, the range of manipulated variables should be specified well until the saturation point of measure variables is observed. This situation is testified from the feed stage location of distillation column 1. Besides that, the range of limits in the optimization must be around the point of optimum condition in order to prevent deviation of optimum conditions.

In this study, optimization parameters involved for this acrylic acid plant are number of stages, solvent flow rate, reflux ratio, feed trays location and reboiler heat duty. They are not only the parameters that can be used for optimization. For the future works, the operating and design cost can be consider for optimization parameters. One of the purposes of optimization is to improve and enhance the operation condition so that can realize the maximum profit. The profit usually based on revenue, raw material cost, operating cost, separation unit cost and heat exchanger network cost. Therefore, this shows that operating and design cost are another good optimization parameters in order to optimize the acrylic acid plant.

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APPENDICES A1

SENSITIVITY BLOCK: R301-T

SAMPLED VARIABLES:
PROIN : PROPY-01MOLEFLOW IN STREAM 7 SUBSTREAM MIXED
ACRY : ACRYL-01MOLEFLOW IN STREAM 8 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=T-SPEC VARIABLE=TEMP ID1=1 IN UOS BLOCK R-301
LOWER LIMIT = 523.0000 K
UPPER LIMIT = 638.0000 K
INCREMENT = 5.0000

FORTRAN STATEMENTS:
YIELD=ACRY/PROIN

TABULATED VARIABLES:
COLUMN 2: YIELD

VARY 1 R-301 1 T-SPEC TEMP K	YIELD
523.0000	0.1568
528.0000	0.1798
533.0000	0.2056
538.0000	0.2346
543.0000	0.2670
548.0000	0.3031
553.0000	0.3433
558.0000	0.3880
563.0000	0.4376
568.0000	0.4925
573.0000	0.5531
578.0000	0.6199
583.0000	0.6934
588.0000	0.7728
593.0000	0.7616
598.0000	0.7501
603.0000	0.7385
608.0000	0.7266
613.0000	0.7101
618.0000	0.6874
623.0000	0.6651
628.0000	0.6435
633.0000	0.6218
638.0000	0.6009
583.1500	0.6957

w WARNINGS OCCURRED FOR VALUES IN THIS ROW.
SEE THE HISTORY FILE FOR DETAILS.

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
PROIN	127.000	KMOL/HR
ACRY	88.3517	KMOL/HR

APPENDICES A2

SENSITIVITY BLOCK: T301-P WITH TEMPERATURE 10 ℃

SAMPLED VARIABLES:
ACRY : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK T-301
LOWER LIMIT = 5.0663+04 N/SQM
UPPER LIMIT = 1.0133+06 N/SQM
INCREMENT = 5.0663+04

FORTRAN STATEMENTS:
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100

TABULATED VARIABLES:
COLUMN 2: REACRY
COLUMN 3: REACET

VARY 1 T-301 PARAM PRES N/SQM	REACRY	REACET
5.0663+04	98.8815	98.8561
1.0133+05	99.4559	99.4334
1.5199+05	99.6430	99.6216
2.0265+05	99.7355	99.7151
2.5331+05	99.7907	99.7709
3.0398+05	99.8272	99.8080
3.5464+05	99.8531	99.8345
4.0530+05	99.8724	99.8543
4.5596+05	99.8874	99.8697

```
!  5.0663+05 !    99.8993 !    99.8820 !
!------------+------------+------------!
!  5.5729+05 !    99.9090 !    99.8921 !
!  6.0795+05 !    99.9170 !    99.9005 !
!  6.5861+05 !    99.9238 !    99.9076 !
!  7.0928+05 !    99.9296 !    99.9137 !
!  7.5994+05 !    99.9346 !    99.9190 !
!------------+------------+------------!
!  8.1060+05 !    99.9389 !    99.9236 !
!  8.6126+05 !    99.9427 !    99.9277 !
!  9.1192+05 !    99.9461 !    99.9313 !
!  9.6259+05 !    99.9491 !    99.9346 !
!  1.0133+06 !    99.9518 !    99.9375 !
!------------+------------+------------!
!  2.4000+05 !    99.7785 !    99.7585 !
----------------------------------------
```

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	88.1560	KMOL/HR
TACRY	88.3517	KMOL/HR
ACET	6.52543	KMOL/HR
TACET	6.54122	KMOL/HR

APPENDICES A3

SENSITIVITY BLOCK: T301-P WITH TEMPERATURE 25 ℃

SAMPLED VARIABLES:
- ACRY : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
- TACRY : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
- ACET : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
- TACET : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

VARIED VARIABLES:

VARY 1: SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK T-301
- LOWER LIMIT = 5.0663+04 N/SQM
- UPPER LIMIT = 1.0133+06 N/SQM
- INCREMENT = 5.0663+04

FORTRAN STATEMENTS:

```
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
```

TABULATED VARIABLES:
- COLUMN 2: REACRY
- COLUMN 3: REACET

```
----------------------------------------
!  VARY 1   !  REACRY   !  REACET   !
```

T-301		
PARAM		
PRES		
N/SQM		
5.0663+04	96.7687	96.9399
1.0133+05	98.4591	98.5298
1.5199+05	98.9927	99.0286
2.0265+05	99.2540	99.2725
2.5331+05	99.4088	99.4172
3.0398+05	99.5111	99.5130
3.5464+05	99.5837	99.5811
4.0530+05	99.6378	99.6320
4.5596+05	99.6797	99.6714
5.0663+05	99.7130	99.7029
5.5729+05	99.7401	99.7287
6.0795+05	99.7627	99.7501
6.5861+05	99.7816	99.7682
7.0928+05	99.7978	99.7837
7.5994+05	99.8118	99.7971
8.1060+05	99.8240	99.8088
8.6126+05	99.8348	99.8192
9.1192+05	99.8443	99.8283
9.6259+05	99.8528	99.8366
1.0133+06	99.8604	99.8439
2.4000+05	99.3745	99.3853

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	87.7991	KMOL/HR
TACRY	88.3517	KMOL/HR
ACET	6.50101	KMOL/HR
TACET	6.54122	KMOL/HR

APPENDICES A4

SENSITIVITY BLOCK: T301-P WITH TEMPERATURE 40 ℃

SAMPLED VARIABLES:
ACRY : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK T-301
LOWER LIMIT = 5.0663+04 N/SQM
UPPER LIMIT = 1.0133+06 N/SQM
INCREMENT = 5.0663+04

FORTRAN STATEMENTS:
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100

TABULATED VARIABLES:
COLUMN 2: REACRY
COLUMN 3: REACET

VARY 1 T-301 PARAM PRES N/SQM	REACRY	REACET
5.0663+04	91.0684	91.9588
1.0133+05	95.9835	96.4157
1.5199+05	97.4168	97.6856
2.0265+05	98.0996	98.2866
2.5331+05	98.4989	98.6371
3.0398+05	98.7607	98.8667
3.5464+05	98.9454	99.0287
4.0530+05	99.0827	99.1492
4.5596+05	99.1886	99.2423
5.0663+05	99.2728	99.3163
5.5729+05	99.3413	99.3767
6.0795+05	99.3980	99.4268
6.5861+05	99.4459	99.4690
7.0928+05	99.4867	99.5052
7.5994+05	99.5219	99.5364
8.1060+05	99.5526	99.5637
8.6126+05	99.5796	99.5877
9.1192+05	99.6035	99.6090
9.6259+05	99.6248	99.6281
1.0133+06	99.6439	99.6452

! 2.4000+05 ! 98.4110 ! 98.5601 !

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	86.9478	KMOL/HR
TACRY	88.3517	KMOL/HR
ACET	6.44703	KMOL/HR
TACET	6.54122	KMOL/HR

APPENDICES A5

SENSITIVITY BLOCK: T301-P WITH TEMPERATURE 55 ℃

SAMPLED VARIABLES:
- ACRY : ACRYL-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
- TACRY : ACRYL-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED
- ACET : ACETI-01MOLEFLOW IN STREAM 13 SUBSTREAM MIXED
- TACET : ACETI-01MOLEFLOW IN STREAM 9 SUBSTREAM MIXED

VARIED VARIABLES:

VARY 1: SENTENCE=PARAM VARIABLE=PRES IN UOS BLOCK T-301
- LOWER LIMIT = 5.0663+04 N/SQM
- UPPER LIMIT = 1.0133+06 N/SQM
- INCREMENT = 5.0663+04

FORTRAN STATEMENTS:

```
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
```

TABULATED VARIABLES:
- COLUMN 2: REACRY
- COLUMN 3: REACET

VARY 1 T-301 PARAM PRES N/SQM	REACRY	REACET
5.0663+04	73.3789	75.9433
1.0133+05	89.8532	91.3257
1.5199+05	93.7360	94.6891
2.0265+05	95.4750	96.1637
2.5331+05	96.4605	96.9917
3.0398+05	97.0951	97.5220

```
!  3.5464+05 !    97.5377 !    97.8907 !
!  4.0530+05 !    97.8638 !    98.1618 !
!  4.5596+05 !    98.1139 !    98.3696 !
!  5.0663+05 !    98.3118 !    98.5339 !
!------------+------------+------------!
!  5.5729+05 !    98.4722 !    98.6671 !
!  6.0795+05 !    98.6048 !    98.7772 !
!  6.5861+05 !    98.7162 !    98.8698 !
!  7.0928+05 !    98.8111 !    98.9487 !
!  7.5994+05 !    98.8928 !    99.0167 !
!------------+------------+------------!
!  8.1060+05 !    98.9640 !    99.0760 !
!  8.6126+05 !    99.0265 !    99.1282 !
!  9.1192+05 !    99.0819 !    99.1743 !
!  9.6259+05 !    99.1312 !    99.2155 !
!  1.0133+06 !    99.1754 !    99.2525 !
!------------+------------+------------!
!  2.4000+05 !    96.2452 !    96.8115 !
-----------------------------------------
```

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	85.0343	KMOL/HR
TACRY	88.3517	KMOL/HR
ACET	6.33266	KMOL/HR
TACET	6.54122	KMOL/HR

APPENDICES A6

SENSITIVITY BLOCK: T302-WAT

SAMPLED VARIABLES:
- WATER : WATER MOLEFLOW IN STREAM 11 SUBSTREAM MIXED
- ACRY : ACRYL-01MOLEFLOW IN STREAM 14 SUBSTREAM MIXED
- TACRY : ACRYL-01MOLEFLOW IN STREAM 10 SUBSTREAM MIXED
- ACET : ACETI-01MOLEFLOW IN STREAM 14 SUBSTREAM MIXED
- TACET : ACETI-01MOLEFLOW IN STREAM 10 SUBSTREAM MIXED

VARIED VARIABLES:
- VARY 1: WATER MOLEFLOW IN STREAM 11 SUBSTREAM MIXED
  - LOWER LIMIT = 2.7778-03 KMOL/SEC
  - UPPER LIMIT = 5.5556-02 KMOL/SEC
  - INCREMENT = 2.7778-03

FORTRAN STATEMENTS:

```
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
```

TABULATED VARIABLES:
- COLUMN 2: REACRY
- COLUMN 3: REACET

```
----------------------------------------
! VARY 1   ! REACRY   ! REACET   !
! 11       !         !         !
! MIXED    !         !         !
! WATER MO !         !         !
! LEFLOW   !         !         !
! KMOL/SEC !         !         !
!         !         !         !
!============!============!============!
!e 2.7778-03 !   18.6288 !    8.7869 !
! 5.5556-03 !   61.3414 !   71.3113 !
! 8.3333-03 !   79.7039 !   91.6587 !
! 1.1111-02 !   89.2782 !   97.0930 !
! 1.3889-02 !   94.1759 !   98.7302 !
!------------+------------+------------!
! 1.6667-02 !   96.7006 !   99.3412 !
! 1.9444-02 !   98.0346 !   99.6138 !
! 2.2222-02 !   98.7570 !   99.7505 !
! 2.5000-02 !   99.1684 !   99.8265 !
! 2.7778-02 !   99.4153 !   99.8723 !
!------------+------------+------------!
! 3.0556-02 !   99.5710 !   99.9018 !
! 3.3333-02 !   99.6736 !   99.9217 !
! 3.6111-02 !   99.7439 !   99.9358 !
! 3.8889-02 !   99.7938 !   99.9461 !
! 4.1667-02 !   99.8299 !   99.9538 !
!------------+------------+------------!
! 4.4444-02 !   99.8574 !   99.9598 !
! 4.7222-02 !   99.8784 !   99.9646 !
! 5.0000-02 !   99.8949 !   99.9684 !
! 5.2778-02 !   99.9080 !   99.9715 !
! 5.5556-02 !   99.9186 !   99.9741 !
!------------+------------+------------!
! 3.9167-02 !   99.7980 !   99.9470 !
----------------------------------------

 e ERRORS OCCURRED FOR VALUES IN THIS ROW.
     SEE THE HISTORY FILE FOR DETAILS.

  VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
    VARIABLE         VALUE        UNITS
    --------         -----        -----
    WATER             141.000       KMOL/HR
    ACRY             1.40109       KMOL/HR
    TACRY             1.40393       KMOL/HR
    ACET            0.941394E-01    KMOL/HR
    TACET            0.941894E-01    KMOL/HR
```

APPENDICES A7

SENSITIVITY BLOCK: T303-DSO

SAMPLED VARIABLES:
ACRY : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 15 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 15 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: DIISO-01MOLEFLOW IN STREAM 16 SUBSTREAM MIXED
LOWER LIMIT = 1.3889-02 KMOL/SEC
UPPER LIMIT = 0.5556 KMOL/SEC
INCREMENT = 1.3889-02

FORTRAN STATEMENTS:
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100

TABULATED VARIABLES:
COLUMN 2: REACRY
COLUMN 3: REACET

VARY 1 MIXED DIISO-01 MOLEFLOW KMOL/SEC	REACRY	REACET
1.3889-02	54.3412	17.9987
2.7778-02	93.3571	32.2667
4.1667-02	98.4433	37.0910
5.5556-02	99.7452	41.0906
6.9444-02	99.9686	44.7944
8.3333-02	99.9961	48.5211
9.7222-02	99.9994	52.3072
0.1111	99.9999	56.1125
0.1250	100.0000	59.9945
0.1389	100.0000	63.8515
0.1528	100.0000	67.8066
0.1667	100.0000	71.7267
0.1806	100.0000	75.6786
0.1944	100.0000	79.5365
0.2083	100.0000	83.3035
0.2222	100.0000	86.8868
0.2361	100.0000	89.9965
0.2500	100.0000	92.7733
0.2639	100.0000	94.8782
0.2778	100.0000	96.5342

```
!     0.2917 !   100.0000 !    97.7181 !
!     0.3056 !   100.0000 !    98.5352 !
!     0.3194 !   100.0000 !    99.0519 !
!     0.3333 !   100.0000 !    99.4017 !
!     0.3472 !   100.0000 !    99.6168 !
!------------+------------+------------!
!     0.3611 !   100.0000 !    99.7569 !
!     0.3750 !   100.0000 !    99.8452 !
!     0.3889 !   100.0000 !    99.9025 !
!     0.4028 !   100.0000 !    99.9360 !
!     0.4167 !   100.0000 !    99.9586 !
!------------+------------+------------!
!     0.4306 !   100.0000 !    99.9729 !
!     0.4444 !   100.0000 !    99.9821 !
!     0.4583 !   100.0000 !    99.9881 !
!     0.4722 !   100.0000 !    99.9919 !
!     0.4861 !   100.0000 !    99.9946 !
!------------+------------+------------!
!     0.5000 !   100.0000 !    99.9962 !
!     0.5139 !   100.0000 !    99.9975 !
!     0.5278 !   100.0000 !    99.9982 !
!     0.5417 !   100.0000 !    99.9987 !
!     0.5556 !   100.0000 !    99.9991 !
!------------+------------+------------!
!     0.3611 !   100.0000 !    99.7603 !
----------------------------------------

 e ERRORS OCCURRED FOR VALUES IN THIS ROW.
     SEE THE HISTORY FILE FOR DETAILS.

  VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
    VARIABLE         VALUE        UNITS
    --------         -----        -----
    ACRY            88.3489       KMOL/HR
    TACRY           88.3489       KMOL/HR
    ACET            6.52549       KMOL/HR
    TACET           6.54117       KMOL/HR
```

APPENDICES A8

SENSITIVITY BLOCK: T304-FS

SAMPLED VARIABLES:
ACRY : ACRYL-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
DSO : DIISO-01MOLEFLOW IN STREAM 19 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TDSO : DIISO-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=FEEDS VARIABLE=STAGE ID1=18 IN UOS BLOCK T-304
LOWER LIMIT = 1.0000
UPPER LIMIT = 15.0000
INCREMENT = 1.0000

FORTRAN STATEMENTS:
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
REDSO=DSO/TDSO*100

TABULATED VARIABLES:
COLUMN 2: REACRY
COLUMN 3: REACET
COLUMN 4: REDSO

VARY 1 T-304 18 FEEDS STAGE	REACRY	REACET	REDSO
1.0000	73.1152	70.1137	97.9296
2.0000	96.9489	92.1990	99.6658
3.0000	99.4161	96.8779	99.8576
4.0000	99.8805	98.6732	99.8983
5.0000	99.9753	99.4295	99.9086
6.0000	99.9949	99.7533	99.9115
7.0000	99.9989	99.8928	99.9125
8.0000	99.9998	99.9525	99.9129
9.0000	100.0000	99.9780	99.9130
10.0000	100.0000	99.9885	99.9131
11.0000	100.0000	99.9925	99.9132
12.0000	100.0000	99.9935	99.9137
13.0000	100.0000	99.9929	99.9170
14.0000	100.0000	99.9913	99.9371
15.0000	100.0000	99.9844	99.9537
4.0000	99.8805	98.6732	99.8983

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	88.2434	KMOL/HR
ACET	6.43897	KMOL/HR
DSO	1294.45	KMOL/HR
TACRY	88.3489	KMOL/HR
TACET	6.52549	KMOL/HR
TDSO	1295.77	KMOL/HR

APPENDICES A9

SENSITIVITY BLOCK: T304-RD

SAMPLED VARIABLES:

ACRY : ACRYL-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
DSO : DIISO-01MOLEFLOW IN STREAM 19 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TDSO : DIISO-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED

VARIED VARIABLES:

VARY 1: SENTENCE=COL-SPECS VARIABLE=QN IN UOS BLOCK T-304
LOWER LIMIT = 1.1111+07 WATT
UPPER LIMIT = 8.3333+07 WATT
INCREMENT = 5.5556+06

FORTRAN STATEMENTS:

```
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
REDSO=DSO/TDSO*100
```

TABULATED VARIABLES:

COLUMN 2: REACRY
COLUMN 3: REACET
COLUMN 4: REDSO

VARY 1 T-304 COL-SPEC QN WATT	REACRY	REACET	REDSO
1.1111+07	91.0828	76.9911	99.1892
1.6667+07	98.7302	90.7617	99.7800
2.2222+07	99.3710	94.3728	99.8418
2.7778+07	99.5843	95.9567	99.8644

```
!  3.3333+07 !    99.6889 !    96.8359 !   99.8759 !
!------------+------------+------------+------------!
!  3.8889+07 !    99.7509 !    97.3956 !   99.8830 !
!  4.4444+07 !    99.7920 !    97.7839 !   99.8877 !
!  5.0000+07 !    99.8212 !    98.0695 !   99.8912 !
!  5.5556+07 !    99.8432 !    98.2887 !   99.8937 !
!  6.1111+07 !    99.8602 !    98.4624 !   99.8958 !
!------------+------------+------------+------------!
!  6.6667+07 !    99.8739 !    98.6035 !   99.8974 !
!  7.2222+07 !    99.8850 !    98.7206 !   99.8988 !
!  7.7778+07 !    99.8943 !    98.8193 !   99.8999 !
!  8.3333+07 !    99.9023 !    98.9038 !   99.9009 !
-----------------------------------------------------
```

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	0.244002E-01	KMOL/SEC
ACET	0.659849E-03	KMOL/SEC
DSO	0.359937	KMOL/SEC
TACRY	0.245414E-01	KMOL/SEC
TACET	0.181264E-02	KMOL/SEC
TDSO	0.359937	KMOL/SEC

APPENDICES A10

SENSITIVITY BLOCK: T304-RR

SAMPLED VARIABLES:

ACRY : ACRYL-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
ACET : ACETI-01MOLEFLOW IN STREAM 20 SUBSTREAM MIXED
DSO : DIISO-01MOLEFLOW IN STREAM 19 SUBSTREAM MIXED
TACRY : ACRYL-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TACET : ACETI-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED
TDSO : DIISO-01MOLEFLOW IN STREAM 18 SUBSTREAM MIXED

VARIED VARIABLES:

VARY 1: SENTENCE=COL-SPECS VARIABLE=MOLE-RR IN UOS BLOCK T-304
LOWER LIMIT = 0.5000
UPPER LIMIT = 10.0000
INCREMENT = 0.5000

FORTRAN STATEMENTS:

```
REACRY=ACRY/TACRY*100
REACET=ACET/TACET*100
REDSO=DSO/TDSO*100
```

TABULATED VARIABLES:

COLUMN 2: REACRY
COLUMN 3: REACET
COLUMN 4: REDSO

VARY 1 T-304 COL-SPEC MOLE-RR	REACRY	REACET	REDSO
0.5000	99.2721	93.7175	99.8319
1.0000	99.6445	96.4531	99.8711
1.5000	99.7636	97.5139	99.8845
2.0000	99.8222	98.0790	99.8914
2.5000	99.8572	98.4316	99.8955
3.0000	99.8805	98.6732	99.8983
3.5000	99.8972	98.8496	99.9003
4.0000	99.9098	98.9840	99.9019
4.5000	99.9196	99.0900	99.9031
5.0000	99.9275	99.1759	99.9040
5.5000	99.9339	99.2468	99.9048
6.0000	99.9393	99.3064	99.9055
6.5000	99.9439	99.3572	99.9061
7.0000	99.9478	99.4010	99.9066
7.5000	99.9512	99.4391	99.9070
8.0000	99.9542	99.4727	99.9074
8.5000	99.9569	99.5025	99.9077
9.0000	99.9592	99.5290	99.9080
9.5000	99.9613	99.5529	99.9082
10.0000	99.9632	99.5744	99.9085
3.0000	99.8806	98.6741	99.8983

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRY	0.245121E-01	KMOL/SEC
ACET	0.178860E-02	KMOL/SEC
DSO	0.359571	KMOL/SEC
TACRY	0.245414E-01	KMOL/SEC
TACET	0.181264E-02	KMOL/SEC
TDSO	0.359937	KMOL/SEC

APPENDICES A11

SENSITIVITY BLOCK: T305-FS

SAMPLED VARIABLES:
ACRYB : ACRYL-01MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
ACETT : ACETI-01MOLEFLOW IN STREAM 21 SUBSTREAM MIXED
TOTALB : TOTAL MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
TOTALT : TOTAL MOLEFLOW IN STREAM 21 SUBSTREAM MIXED

VARIED VARIABLES:
VARY 1: SENTENCE=FEEDS VARIABLE=STAGE ID1=20 IN UOS BLOCK T-305
LOWER LIMIT = 2.0000
UPPER LIMIT = 36.0000
INCREMENT = 1.0000

FORTRAN STATEMENTS:
PUR1=ACRYB/TOTALB*100
PUR2=ACETT/TOTALT*100

TABULATED VARIABLES:
COLUMN 2: PUR1
COLUMN 3: PUR2

VARY 1 T-305 20 FEEDS STAGE	PUR1	PUR2
2.0000	97.2164	48.0529
3.0000	98.5368	62.5768
4.0000	99.3339	71.3448
5.0000	99.7447	75.8638
6.0000	99.9252	77.8493
7.0000	99.9911	78.5740
8.0000	99.9984	78.6550
9.0000	99.9991	78.6626
10.0000	99.9993	78.6643
11.0000	99.9992	78.6638
12.0000	99.9990	78.6619
13.0000	99.9988	78.6586
14.0000	99.9984	78.6539
15.0000	99.9977	78.6470
16.0000	99.9969	78.6374
17.0000	99.9956	78.6240
18.0000	99.9940	78.6054
19.0000	99.9916	78.5796
20.0000	99.9883	78.5437
21.0000	99.9838	78.4941
22.0000	99.9775	78.4254
23.0000	99.9690	78.3304

```
!   24.0000 !   99.9570 !   78.1991 !
!   25.0000 !   99.9405 !   78.0180 !
!   26.0000 !   99.9178 !   77.7683 !
!-----------+-----------+-----------!
!   27.0000 !   99.8866 !   77.4243 !
!   28.0000 !   99.8435 !   76.9504 !
!   29.0000 !   99.7841 !   76.2966 !
!   30.0000 !   99.7018 !   75.3919 !
!   31.0000 !   99.5874 !   74.1331 !
!-----------+-----------+-----------!
!   32.0000 !   99.4264 !   72.3627 !
!   33.0000 !   99.1959 !   69.8306 !
!   34.0000 !   98.8557 !   66.1126 !
!   35.0000 !   98.3230 !   60.4206 !
!   36.0000 !   97.3770 !   51.1087 !
!-----------+-----------+-----------!
!   23.0000 !   99.9689 !   78.3304 !
----------------------------------------
```

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRYB	87.9687	KMOL/HR
ACETT	6.40763	KMOL/HR
TOTALB	88.0000	KMOL/HR
TOTALT	8.00000	KMOL/HR

APPENDICES A12

SENSITIVITY BLOCK: T305-RD

SAMPLED VARIABLES:
- ACRYB : ACRYL-01MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
- ACETT : ACETI-01MOLEFLOW IN STREAM 21 SUBSTREAM MIXED
- TOTALB : TOTAL MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
- TOTALT : TOTAL MOLEFLOW IN STREAM 21 SUBSTREAM MIXED

VARIED VARIABLES:

VARY 1: SENTENCE=COL-SPECS VARIABLE=QN IN UOS BLOCK T-305
- LOWER LIMIT = 5.5556+04 WATT
- UPPER LIMIT = 8.3334+05 WATT
- INCREMENT = 5.5556+04

FORTRAN STATEMENTS:

```
PUR1=ACRYB/TOTALB*100
PUR2=ACETT/TOTALT*100
```

TABULATED VARIABLES:
- COLUMN 2: PUR1
- COLUMN 3: PUR2

```
----------------------------------------
! VARY 1    ! PUR1     ! PUR2     !
! T-305     !          !          !
! COL-SPEC  !          !          !
! QN        !          !          !
!          !          !          !
! WATT      !          !          !
!          !          !          !
!============!============!============!
! 5.5556+04 !   93.9580 !   14.1543 !
! 1.1111+05 !   94.3239 !   18.0517 !
! 1.6667+05 !   95.1382 !   27.0038 !
! 2.2222+05 !   95.9523 !   35.9584 !
! 2.7778+05 !   96.7641 !   44.8884 !
!------------+------------+------------!
! 3.3334+05 !   97.5633 !   53.6804 !
! 3.8889+05 !   98.3175 !   61.9762 !
! 4.4445+05 !   98.9601 !   69.0442 !
! 5.0000+05 !   99.4192 !   74.0950 !
! 5.5556+05 !   99.6899 !   77.0728 !
!------------+------------+------------!
! 6.1112+05 !   99.8321 !   78.6371 !
! 6.6667+05 !   99.9055 !   79.4438 !
! 7.2223+05 !   99.9439 !   79.8662 !
! 7.7778+05 !   99.9651 !   80.0996 !
! 8.3334+05 !   99.9774 !   80.2345 !
!------------+------------+------------!

 e ERRORS OCCURRED FOR VALUES IN THIS ROW.
     SEE THE HISTORY FILE FOR DETAILS.

 VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
   VARIABLE         VALUE        UNITS
   --------        -----        -----
   ACRYB          0.266667E-06    KMOL/SEC
   ACETT          0.179771E-02    KMOL/SEC
   TOTALB         0.266667E-06    KMOL/SEC
   TOTALT         0.266664E-01    KMOL/SEC
```

APPENDICES A13

SENSITIVITY BLOCK: T305-RR

```
 SAMPLED VARIABLES:
   ACRYB    : ACRYL-01MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
   ACETT    : ACETI-01MOLEFLOW IN STREAM 21 SUBSTREAM MIXED
   TOTALB   : TOTAL MOLEFLOW IN STREAM 22 SUBSTREAM MIXED
   TOTALT   : TOTAL MOLEFLOW IN STREAM 21 SUBSTREAM MIXED

 VARIED VARIABLES:
   VARY    1: SENTENCE=COL-SPECS VARIABLE=MOLE-RR IN UOS BLOCK T-305
```

LOWER LIMIT = 1.0000
UPPER LIMIT = 15.0000
INCREMENT = 1.0000

FORTRAN STATEMENTS:
PUR1=ACRYB/TOTALB*100
PUR2=ACETT/TOTALT*100

TABULATED VARIABLES:
COLUMN 2: PUR1
COLUMN 3: PUR2

VARY 1 T-305 COL-SPEC MOLE-RR	PUR1	PUR2
1.0000	95.0270	23.9699
2.0000	95.9584	34.2150
3.0000	96.8446	43.9633
4.0000	97.6756	53.1046
5.0000	98.4203	61.2959
6.0000	99.0278	67.9789
7.0000	99.4549	72.6764
8.0000	99.7090	75.4715
9.0000	99.8439	76.9556
10.0000	99.9132	77.7180
11.0000	99.9493	78.1147
12.0000	99.9689	78.3306
13.0000	99.9801	78.4535
14.0000	99.9867	78.5266
15.0000	99.9909	78.5719
12.0000	99.9689	78.3306

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
ACRYB	0.244357E-01	KMOL/SEC
ACETT	0.177990E-02	KMOL/SEC
TOTALB	0.244444E-01	KMOL/SEC
TOTALT	0.222222E-02	KMOL/SEC