# Production of 22,000 Tons/Yr. of Vinyl Acetate Monomer by Oxy-Acetylation of Ethylene

*By*

Muhammad Saad Chaudhary, FA19-CHE-022
Muhammad Faizan, FA19-CHE-038
Shehryar Niazi, FA19-CHE-064
Affan Bin Zahid, FA19-CHE-080
Muhammad Saqib Bashir, FA19-CHE-084

COMSATS University Islamabad
Lahore Campus - Pakistan

Spring, 2023

COMSATS University Islamabad, Lahore Campus

# Production of 22,000 Ton/Yr. of Vinyl Acetate Monomer by Oxy-Acetylation of Ethylene

A Chemical Engineering Plant Design Project Report Presented to

**COMSATS University Islamabad**

In partial fulfillment

of the requirement for the degree of

**Bachelor of Science in Chemical Engineering**

*By*

| Name: | Registration ID. |
|---|---|
| Muhammad Saad Chaudhary | FA19-CHE-022 |
| Muhammad Faizan | FA19-CHE-038 |
| Shehryar Niazi | FA19-CHE-064 |
| Affan Bin Zahid | FA19-CHE-080 |
| Muhammad Saqib | FA19-CHE-084 |

Spring, 2023

# Production of 22,000 Ton/Yr. of Vinyl Acetate Monomer by Oxy-Acetylation of Ethylene

The Department of Chemical Engineering received a Chemical Engineering Plant Design Project Report as partial fulfilment of the requirement for the degree of Bachelor of Science in Chemical Engineering.

| Name | Registration ID. |
|---|---|
| Muhammad Saad Chaudhary | FA19-CHE-022 |
| Muhammad Faizan | FA19-CHE-038 |
| Shehryar Niazi | FA19-CHE-064 |
| Affan Bin Zahid | FA19-CHE-080 |
| Muhammad Saqib Bashir | FA19-CHE-084 |

**Supervisor**

Dr. Mehwish Batool

Assistant Professor

Department of Chemical Engineering,

COMSATS University Islamabad, Lahore campus.

# Author’s Declaration

We now declare that our Chemical Engineering Plant Design Report, "Production of 22,000 Tons/Year of Vinyl Acetate Monomer by Oxy-Acetylation of Ethylene," and all information included in the references, are our original work. This report has never before been submitted by us for the purpose of obtaining a degree from COMSATS University Islamabad or any other university.

Name: Muhammad Saad Chaudhary
Signature: ____________________

Name: Shehryar Niazi
Signature: _________________

Name: Affan Bin Zahid
Signature: ____________________

Name: Muhammad Saqib Bashir
Signature: __________________

Name: Muhammad Faizan
Signature: _____________

May 26, 2023

# **Supervisor’s Declaration**

We hereby certify that we have read this thesis and that, in our judgement, it meets the requirements for the award of the degree of Bachelor of Chemical Engineering in terms of scope and quality.

Name: Dr. Mehwish Batool

Signature: ______________

# DEDICATION

We are grateful to Allah Almighty for the knowledge, guidance, and protection that helped us complete our Chemical Engineering project. We also want to express our heartfelt appreciation to our FYDP supervisor, Dr. Mehwish Batool, for her valuable time, effort, and patience in guiding us throughout the project. We are grateful for her insights, encouragement, and support, which have helped us understand the subject matter and complete this project successfully.

Additionally, we dedicate this project to our parents, whose unwavering support and encouragement have been our constant source of inspiration and strength. Their moral, emotional, spiritual, and financial support have helped us overcome the challenges and obstacles we faced during this project. We owe our success to them. We would also like to extend our appreciation to our teachers.

# ACKNOWLEDGEMENTS

We'd like to take this opportunity to acknowledge the contributions and support of individuals who have helped us complete this project. First and foremost, we'd like to thank Allah Almighty for granting us the ability to undertake and complete this study. We're thankful for the guidance, protection, and power of mind that He has bestowed upon us.

We'd also like to express our sincere appreciation to our parents, whose unwavering support and encouragement have been our constant source of inspiration and strength. Their moral, emotional, spiritual, and financial support have helped us overcome the challenges and obstacles we faced during this project.

We would like to express our gratitude to our FYDP supervisor, Dr. Mehwish Batool, for her valuable time, effort, and patience in guiding us throughout the project. We are grateful for her insights, encouragement, and support, which have helped us understand the key concepts of Chemical Engineering. We also thank our teachers.

Last but not least, we'd like to thank our classmates and friends who have supported and motivated us throughout this project. Their words of encouragement and advice have kept us focused and motivated. We acknowledge the contributions of all the individuals who have helped us in this journey, and we hope that our work will be useful to the scientific community.

# ABSTRACT

# Production of 22,000 Ton/Yr. of Vinyl Acetate Monomer by Oxy-Acetylation of Ethylene

This project aims to address the growing demand for Vinyl acetate Monomer (VAM) in Pakistan and foster growth in the polymer sector. To achieve this, various methods of producing VAM have been carefully analyzed and evaluated for cost-effectiveness, and Oxy-Acetylation of Ethylene has been determined to be the most efficient and economical approach. This method involves a straightforward process using a catalyst at the appropriate temperature and pressure to produce high-purity VAM.

To design the VAM production plant, several critical steps have been undertaken, including conducting mass and energy balances, designing the primary equipment, developing process instrumentation and control, and estimating the process's cost. The significance of this initiative is its potential to drive growth in the polymer sector in Pakistan, given that this method has been successfully industrialized in other countries.

# TABLE OF CONTENTS

# LIST OF FIGURES

# LIST OF TABLES

# LIST OF ABBREVIATIONS

| | |
|---|---|
| VAM | Vinyl Acetate Monomer |
| PVA | Poly-vinyl Acetate |
| EVA | Ethylene Vinyl Acetate |
| Pd based | Palladium Based |
| PVOH | Polyvinyl Alcohol |
| PVB | Polyvinyl Butyral |
| EVOH | Ethylene Vinyl Alcohol |
| EDA | Ethylidene diacetate |
| MEA | Mono-ethanol-amine |
| HQ | Hydroquinone |
| $FeCl_3$ | Ferric Chloride |
| $PdCl_2$ | Palladium Dichloride |
| $CuCl_2$ | Cupric Chloride |
| PVAs | Polyvinyl Acetyls |
| BWG | Birmingham Wire Gauge |
| LHV | Lower Heating Value |
| HAZOP | Hazard and Operability Study |
| HAZID | Hazard Identification |

# LIST OF APPENDICES

# Chapter 1

# Introduction

## 1.1. Project Description:

This project is concentrated on the vinyl acetate monomer synthesis process with the intention of starting manufacturing in Pakistan. Many polymeric and polymers products, such as paints, adhesives, binders, moldings, various types of coatings, cosmetics, pharmaceuticals, and numerous more items for use in agriculture, industry, and daily life, all contain vinyl acetate monomer (VAM) as a key chemical constituent. The 22,000 Ton per year of VAM capacity is chosen by taking into account the annual import statistics. Out of all possible manufacturing methods, the oxy-acetylation of ethylene employing a Pd-based catalyst approach was chosen for this project. The reaction has carried out in the plug flow (tubular) reactor.

$$C_2H_4 + CH_3COOH + 0.5\ O_2 \xrightarrow{Pd} C_4H_6O_2 + H_2O$$

Then, employing absorption, distillation, decantation, flash separate key on, and other processes, VAM is separated from the other chemical reaction's constituents. Flashing is mostly used to remove the gaseous byproducts (oxygen, ethylene, and carbon dioxide). VAM is entirely absorbed via absorption, separating from the remaining gaseous components. While VAM is totally recovered from the liquid components (water and acetic acid) via distillation and decantation. While VAM can be produced by three ways:

- By reacting Acetic acid and Acetylene

$$C_2H_2 + CH_3COOH \longrightarrow C_4H_6O_2$$

- By reacting Acetaldehyde and Acetic Anhydride

$$CH_3CHO + (CH_3CO)_2O \longrightarrow C_2H_4\text{-}(OCOCH_3)_2$$

$$C_2H_4\text{-}(OCOCH_3)_2 \longrightarrow C_4H_6O_2 + CH_3COOH$$

- By reacting Acetic acid, Ethylene and oxygen.

$$C_2H_4 + CH_3COOH + 0.5\ O_2 \xrightarrow{Pd} C_4H_6O_2 + H_2O$$

The project's main objective is to develop a chemical engineering solution to a genuine industrial problem while taking Pakistan's economic and marketing environment into consideration. While the project involves the subsequent phases for VAM manufacture.

- Develop a Process Flow Diagram (PFD) using Microsoft Visio.
- Conduct HAZOP analysis.
- Material and Energy balance on the complete process.
- Design Process Equipment (Reactor, Heat exchanger, Liquid-Gas Separator, Absorber, Distillation Column)
- Perform process simulations using suitable software (Aspen HYSYS/Aspen Plus).
- Develop a process instrumentation diagram (P&ID) using MS Visio.
- Conduct a HAZOP study.
- Perform an economic analysis of process.

## 1.2. Background:

Polyvinyl acetate homopolymer (PVA or PVAs) is a significant polymer used in chewing gum, adhesives, and textile sizing. When German chemist Fritz Klatte noticed that vinyl acetate readily interacts with itself, he made the discovery of PVA in 1912. The PVA formulations created by Klatte were solid, dense materials, but over time, researchers discovered ways to create the polymer in different forms. PVA latices are widely used in adhesives. Elmer's Glue is one of the most well-known brands. PVA adhesives are employed in a variety of packaging materials, including bags and shipping boxes, food containers, tapes, binders for foil, envelopes, palstics and paper. Vinyl acetate is coupled with other monomers like ethylene and acrylates to create a variety of copolymers in addition to homopolymers. Ethylene vinyl acetate (EVA) copolymers (also known as EVAs) can be produced in large quantities or using emulsion polymerization. Emulsion EVAs have a variety of applications, including homopolymers of vinyl acetate-like adhesives. Applications for bulk polymers range from high-volume industrial uses to the convenient glue sticks you might have at home or in the classroom **[1].**

## 1.3. Literature Review:

The organic compound vinyl acetate has the following structural formula:

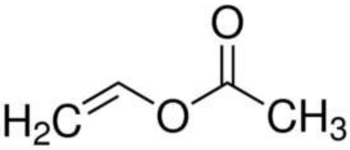


**Figure 1:** Structural formula of VAM

It is a crucial raw material utilized in the production of several goods that form the foundation of the polymer industry. The chemical building block used in the production of a vast array of industrial goods is vinyl acetate. An odorless, flammable liquid with a low flash point, vinyl acetate monomer (VAM) has a distinct taste and color. Vinyl acetate is soluble in the majority of typical organic solvents despite not being soluble in water. A wide range of industrial and consumer applications use polyvinyl acetate homopolymers and copolymers, which are made using vinyl acetate as a precursor **[2].**

### 1.3.1. Physical and thermodynamic properties of VAM:

**Table 1:** Thermodynamic and Physical Properties of VAM [3]

| Properties | Vinyl Acetate |
|---|---|
| **Chemical Formula** | $C_4H_6O_2$ |
| **Appearance** | Colorless Liquid |
| **Molecular Weight (kg/kmol)** | 86.09 |
| **Density (kg/m$^3$)** | 933.8 |
| **Boiling Point (°C)** | 72.9 |
| **Freezing Point (°C)** | -92.8 |
| **Specific Gravity** | 0.934 |
| **Critical temperature (°C)** | 246 |
| **Critical pressure (kPa)** | 3950 |
| **Viscosity at 20 °C** | 0.43 |

### 1.3.2. Application of VAM in Industries:

Though many substances are capable of polymerizing, VAM stands out for how quickly the process can take place in bulk, solution, emulsion, or suspension. VAM is the precursor to each of these consumer products produced through the polymerization processes, but in order to store and distribute them, hydroquinone must be employed as an inhibitor to stop polymerization and the finished product must be chilled **[4]**. The application of VAM involves:

- PVA
- PVOH
- PVB
- EVA
- EVOH
- PVAs

**Table 2:** Applications of VAM in Industries [3]

| **Product Abbreviation** | **Product Name** | **Uses** |
|---|---|---|
| **PVA** | Polyvinyl Acetate | • Paints and Adhesives<br>• Textile Binders<br>• Textile Finishes<br>• Coating for Flexible Substrates<br>• Paper Coating |
| **PVOH** | Polyvinyl Alcohol | • Adhesives<br>• Paper and Textile Coating<br>• Binders for Building Products<br>• Photosensitive Coatings<br>• Moldings<br>• Thickening Agents |
| **PVB** | Polyvinyl Butyral | • Used as a laminated glass for automobiles and commercial<br>• Coatings and inks |
| **EVA** | Ethylene Vinyl Acetate | • Molding<br>• Wires and Cable Coatings<br>• Elastomers<br>• Molded Rubber applications |
| **EVOH** | Ethylene Vinyl Alcohol | • Provide Food barrier<br>• Medical &Pharmaceuticals<br>• Cosmetics<br>• Applications of Packaging in Industrial and Agricultural sector |
| | | • Primers and Adhesives<br>• Metal Coatings |

| | | |
|---|---|---|
| **PVAs** | Polyvinyl Acetyls | • Textile Coatings |

### 1.3.3. Raw Materials:

The raw material for this project is:

- Oxygen
- Acetic Acid
- Ethylene

### 1.3.4. Reaction:

The reaction involved in this process is given as:

$$\mathbf{C_2H_4 + CH_3COOH + 0.5\ O_2 \xrightarrow{Pd} C_4H_6O_2 + H_2O}$$

In this process ethylene and oxygen as a gas and acetic acid as a liquid reacts to produce vinyl acetate and water. This reaction is carried out in the reactor at 147 – 159℃.

While there are two more reactions in which vinyl acetate in produced but oxy-acetylation is economic and better than all the processes.

# Chapter 2

# Market Analysis and Capacity Selection

## 2.1. World VAM Supply and Demand:

The world is quickly transitioning to a plastic economy since we are living in the age of plastics. Plastics and polymeric goods can be found everywhere. Plastics and other polymeric products are included in almost all of the things we use every day.

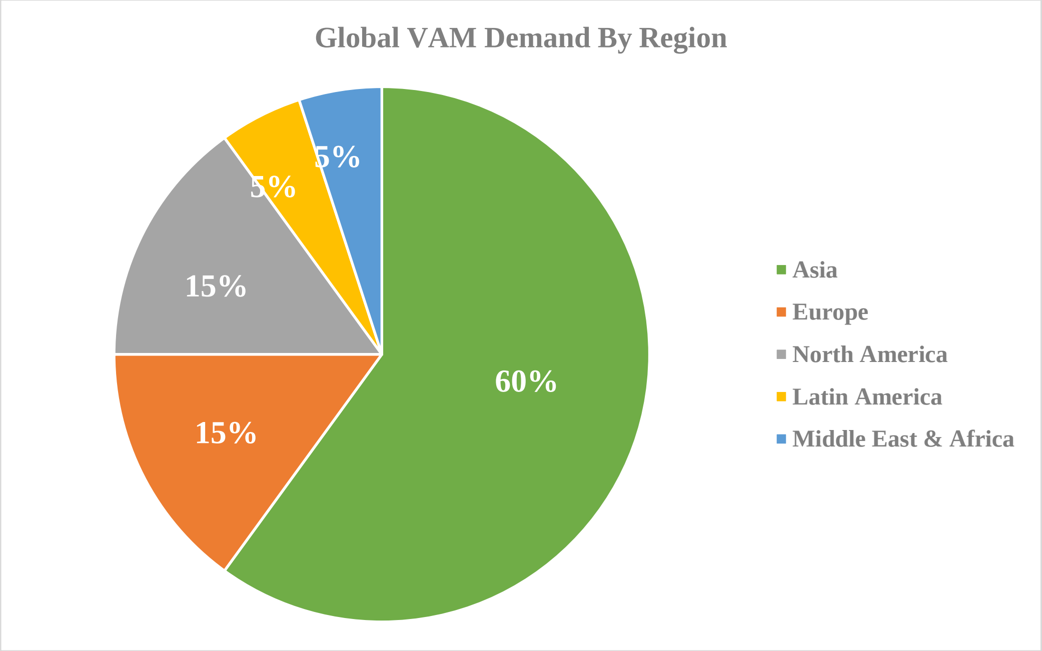


**Figure 2:** Demand of VAM in world by 2021

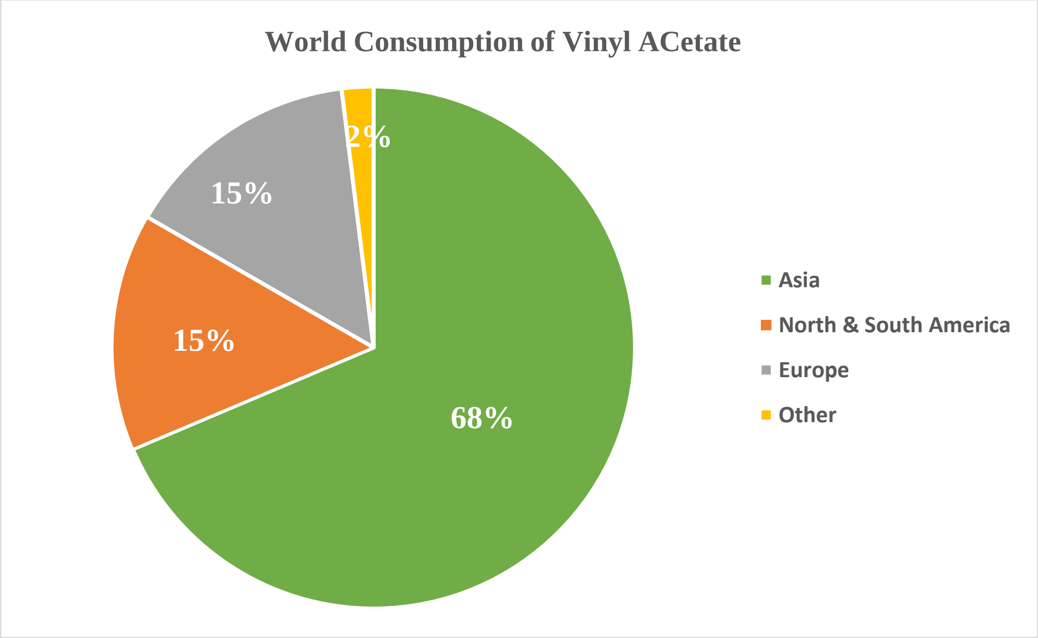


**Figure 3:** Consumption of VAM in world by 2021 [5]

## 2.2. Pakistan’s Annual VAM Consumption:

All of Pakistan's vinyl acetate consumption is dependent on imports from nearby oil-rich countries in the Persian Gulf and the Middle East because vinyl acetate monomer, one of the key components, is required for the creation of numerous valuable polymers and polymeric products. We have selected the production capacity of our project to meet the continually increasing demand for VAM and attain self-sufficiency in VAM manufacture.

The following industries in Pakistan that import VAM:

- Griffon Plastic Industries Limited, Shahdara
- Power Chemical Industries (Pvt.) Limited
- Karachi-based Alsons Auto Parts (Pvt.) Limited
- Lahore-based Neelam Industries
- Karachi-based Arfeen International (Pvt.) Limited

**Table 3:** Annual VAM import of Pakistan

| **Import Year** | **Product** | | | |
|---|---|---|---|---|
| | **Vinyl Acetate Monomer (VAM)** | | | |
| | **Ton/Yr.** | **Ton/day** | **Kg/Yr.** | **Kg/day** |
| **2014** | 14501.45 | 39.73 | 13155494.14 | 36042.44 |
| **2015** | 15136.55 | 41.47 | 13731647.17 | 37620.95 |
| **2016** | 15435.85 | 42.29 | 14003167.56 | 38364.84 |
| **2017** | 16611.15 | 45.51 | 15069381.79 | 41285.97 |
| **2018** | 18191.6 | 49.84 | 16503141.92 | 45214.08 |
| **2019** | 19118.7 | 52.38 | 17344192.89 | 47518.33 |
| **2020** | 19856 | 54.4 | 18013060 | 49350.85 |
| **2021** | 21728.45 | 59.53 | 19711718.26 | 54004.70 |

## 2.3. Capacity Selection:

Given that Pakistan currently imports roughly 23,000 tonnes of VAM annually, it is accurate to state that the country's demand for the substance is growing. As a result, we draw the conclusion that this amount may rise even further in the future year, which could put pressure on the nation's economy. In order to fulfil the rising demand for VAM, we have chosen for our project plant's production capacity to be 22,000 metric tonnes annually.

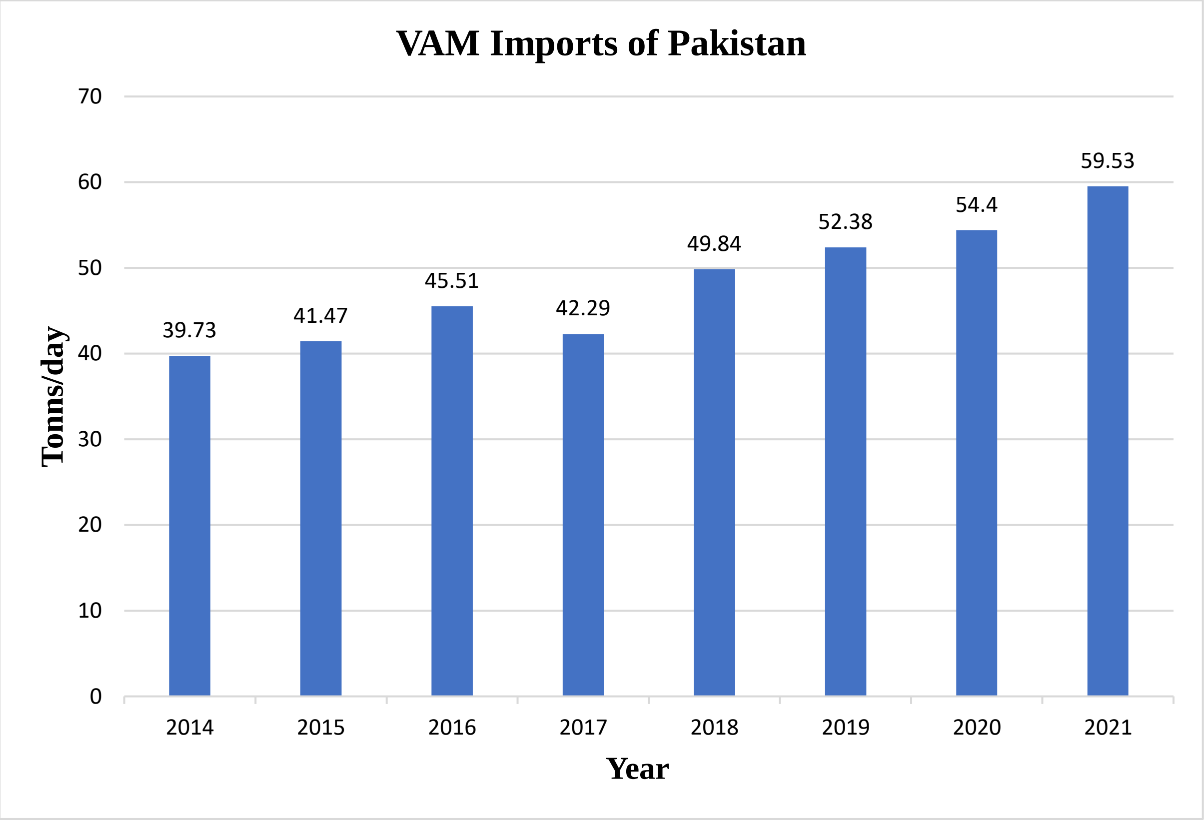


**Figure 4:** Annual VAM Import

## 2.4. Site Location:

The proposed project involves oxy-acetylating ethylene to produce vinyl acetate. Given that Karachi is an industrial and port city, the construction and commissioning of this plant will have a favorable impact on Pakistan's economy as a whole as well as on employment and business prospects. Karachi was chosen because it will be economical to ship imported machinery through its seaport and to regularly provide raw materials. Additionally, Karachi is a center for the polymer sector, making it simple to identify customers for our product, VAM.

# Chapter 3

# Process Selection

## 3.1. Production Processes:

There are three reactions that can be used to create vinyl acetate monomer, and they are as follows:

- VAM is created when acetic acid and acetylene react.
- VAM is created when acetaldehyde and acetic anhydride react.
- VAM is created when acetic acid, ethylene, and oxygen react.

### 3.1.1. Reaction of Acetic Acid and Acetylene

Acetic acid and acetylene are processed using this method by first passing them into a vaporizer, which operates at 170 to 250°C. In order to carry out the addition reaction that results in crude VAM, the reactor comprises a zinc acetate catalyst that has been impregnated on charcoal.

$$\mathbf{C_2H_2 + CH_3COOH \longrightarrow C_4H_6O_2}$$

**[6]**. Acetic acid and acetylene are reacted to form vinyl acetate monomer (VAM) in a vapor-phase process. The reaction mixture is cooled and fed to a flash separator, where the VAM vapor is separated from the unreacted acetylene. The VAM vapor is then fed to a scrubbing column, where it is scrubbed with water to remove any residual acetylene. The scrubbed VAM vapor is then condensed and fed to a light key separation column, where it is separated from any heavier components. The VAM is then fed to a purification column, where it is purified to remove any impurities. The purified VAM is then sent to storage. Acetic acid that hasn't been reacted is recycled back into the vaporizer. **[7]**.

### 3.1.2. Reaction of Acetaldehyde and Acetic Anhydride:

Ethylidene diacetate (EDA) synthesis happens in two steps. Acetaldehyde and acetic anhydride are heated to 120–140 degrees Celsius in a reactor using a $FeCl_3$ catalyst in the first stage. This reaction produces EDA and acetic acid. In the second stage, the EDA is purified by distillation, the following liquid phase reaction occurs:

$$\mathbf{CH_3CHO + (CH_3CO)_2O \longrightarrow C_2H_4(OCOCH_3)_2}$$

Acetaldehyde has an extremely low boiling point of 20 degrees Celsius, which allows it to be easily separated from the other reaction products by flash distillation. The EDA is then recycled or fed to the following stage, as shown, after the EDA and acetic anhydride have been separated in a distillation column:

$$\mathbf{C_2H_4\text{-}(OCOCH_3)_2 \longrightarrow C_4H_6O_2 + CH_3COOH}$$

Acetic acid and VAM can also be flash separated from unreacted EDA and recycled before being fed to separate purification columns to produce the products.

### 3.1.3. Reaction of Acetic Acid, Ethylene and Oxygen:

Acetic acid, ethylene, and oxygen are delivered into a cooled tubular reactor at a temperature of 421 K and 6 Bar, together with a vaporizer running at 7 Bar and 423 K. The subsequent vapor phase reactions take place. **[8]**:

$$\mathbf{C_2H_4 + CH_3COOH + 0.5O_2 \xrightarrow{Pd} C_2H_3OOC_2H_3 + H_2O}$$

$$\textbf{Side Reaction: } \mathbf{C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O}$$

Vinyl acetate monomer (VAM) is produced primarily via a side reaction that also produces carbon dioxide as an unwanted by-product. The cooler, which lowers the temperature to 310 Kelvin, then feeds the reacting gas to a separator. As a result, the separator's VAM, water, and unreacted acetic acid condense. After that, an initial absorption column receives the unreacted ethylene, oxygen, carbon dioxide, and uncondensed VAM. Acetic acid, which serves as a solvent in a wash stream in this column, absorbs the uncondensed VAM. The remaining gas is injected into a second absorption column where the carbon dioxide is removed using mono-ethanol-amine (MEA).

Through the use of a compressor, the remaining gas is recycled to the vaporizer. The de-euthanizer distillation column is where the ethylene is extracted from the VAM crude after each stage. The acetic acid is condensed and recycled to the vaporizer in the azeotropic distillation column from which the column bottoms are supplied. The water is extracted from the aqueous VAM mixture in a decanter and separator. **[1].**

## 3.2. Process Comparison:

The comparison of all the above processes is given as:

**Table 4:** Comparison Table of Different Process

| **Production Processes** | **Acetic Acid and Acetylene** | **Acetaldehyde and Acetic Anhydride** | **Acetic Acid, Ethylene and Oxygen** |
|---|---|---|---|
| **Pressure** | 15 - 18 bar | 20 – 40bar | 9 – 40bar |
| **Temperature** | 170 – 250℃ | 120 – 140℃ | 110 – 160℃ |
| **Catalysts** | Zn $(OAs)_2$ Impregnated on Charcoal | $FeCl_3$ | $PdCl_2$ / $CuCl_2$ (Corrosive)<br>Pd/Au - KOAs impregnated on Silica (2 year) |
| **Economics** | Expensive | Relative Expensive | Expensive and Feasible |
| **Advantages** | Single step process | Renewable raw materials | Better productivity and high conversion per pass |
| **Disadvantages** | Lower conversion per pass | Corrosion problem due to liquid phase reaction | By product $CO_2$ is produced |

Based on the comparison of different production processes for vinyl acetate monomer (VAM), we have selected the oxy-acetylation of ethylene process for our project. This process is relatively efficient and cost-effective, and it produces a high quality product **[9].**

# Chapter 4

# Process Flow Diagram

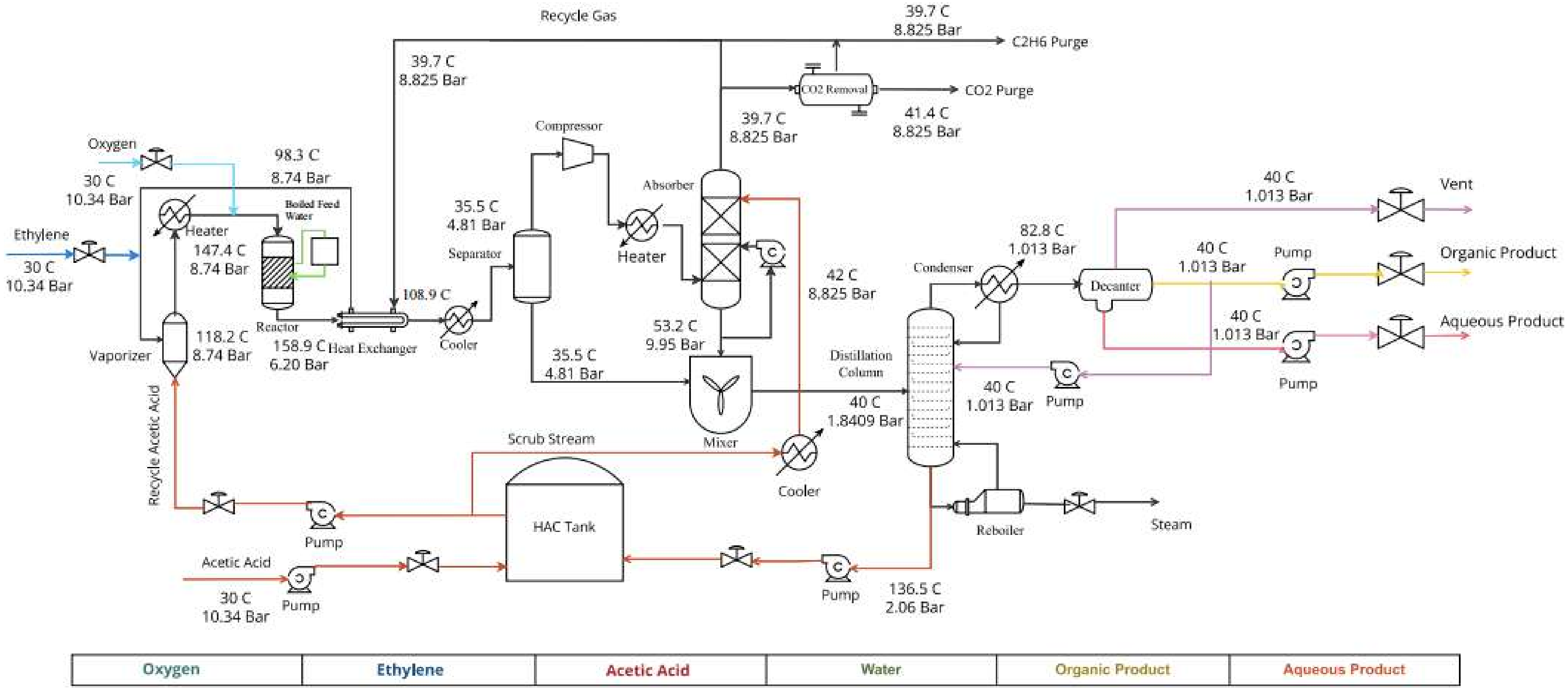


**Figure 5:** Process Flow Diagram of Oxy-Acetylation of Ethylene

## 4.1. Process Description:

The fundamental unit activities for the vinyl acetate production process, which is the subject of this study and the strategy we want to design and implement, are:

- Vaporizer
- Reactor
- Heat Exchanger
- Separator
- Absorber
- Distillation column

### 4.1.1. Reactants:

Our process reaction requires three reactants: oxygen, ethylene, and acetic acid. where acetic acid is a liquid and oxygen and ethylene are gases at normal temperature. Gases are combusted at a pressure of 7 bar, combined with recycled gas from an absorber, and then heated to 150°C in a heat exchanger. Reactants enter the reactor after the acetic acid has been combined with recycling acid from the distillation column, which has been heated to 150°C and vaporized.

### 4.1.2. Vaporizer:

The vaporizer is a heat exchanger that uses steam to heat the feed. The steam heats the feed to its boiling point, which vaporizes the liquid. The vaporized feed is then passed to the heater. The vaporizer is typically a large, cylindrical vessel made of stainless steel. The vessel is equipped with a steam inlet and a liquid feed inlet. The steam inlet is located at the bottom of the vessel, and the liquid feed inlet is located at the top of the vessel. The steam and liquid feed are mixed in the vessel, and the heat from the steam vaporizes the liquid feed. The vaporized feed is then passed out of the vessel through a vapor outlet.

The vaporizer is an important part of the process of producing acetic acid from ethylene and oxygen. The vaporizer ensures that the liquid feed is vaporized before it enters the heater. This is important because the reaction that produces acetic acid occurs in the gas phase. If the liquid feed were not vaporized, it would not be able to react with the oxygen to form acetic acid. The vaporizer is a critical piece of equipment in the production of acetic acid. It ensures that the liquid feed is vaporized before it enters the heater, which is necessary for the reaction that produces acetic acid to occur.

### 4.1.3. Reactor:

Ethylene, oxygen, and acetic acid are the three primary chemical inputs needed to produce VAM. These basic materials are mixed together in a reactor to create the byproducts VAM, water, and carbon dioxide. Ethane is also believed to arrive with the ethylene feed stream as an entrance component. The two reactions listed below are taken into account when creating VAM:

$$\mathbf{C_2H_4 + CH_3COOH + 0.5O_2 \xrightarrow{Pd} C_2H_3OOCCH_3 + H_2O}$$

$$\mathbf{C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O}$$

An exothermic technique is used to create vinyl acetate monomer (VAM) in a reactor with tubes filled with a precious metal catalyst on a silica support. The heat of the reaction is removed by creating steam on the shell side of the tubes. From a steam drum, where make-up water is fed, water enters the reactor. As saturated vapor, the steam emerges from the drum. Under the specified circumstances of 150°C temperature and 7 bar pressure, the reaction takes place and is irreversible. Water, $CO_2$, and vinyl acetate are the reactions end products. Cooling coils are used to reduce the heat generated during chemical reactions because the reactions are strongly exothermic in nature. VAM, carbon dioxide, water, unconverted oxygen, ethylene, and acetic acid are all present in the exit stream.

### 4.1.4. Heat Exchanger:

Using cold steam from the gas recycle, the reactor effluent is cooled in a process-to-process heat exchanger. After cooling with cooling water, the reactor effluent is transferred to a separator. The VAM is separated from the reactor's other components by the separator. Before entering the flash column, the VAM-rich stream from the reactor is cooled using a heat exchanger to 34.5°C and 7 bar of pressure.

### 4.1.5. Flash Separator:

The components of a flash column separate into liquid and gaseous phases when the pressure is reduced to 4 bar. Ethylene, carbon dioxide, and oxygen are among the gases exhaled. Further processing is necessary after collecting VAM from its liquid constituents, including water, acetic acid with a little quantity of oxygen, carbon dioxide, and ethylene.

In a separator, the reaction's vapor and liquid byproducts are separated. The oxygen, ethylene, carbon dioxide, and ethane-containing vapor stream is sent towards a compressor. The liquid stream is directed to the azeotropic distillation column together with vinyl acetate, water, and acetic acid.

### 4.1.6. $CO_2$ Removal System:

This method of eliminating carbon dioxide ($CO_2$) from a gas stream is common in industry. First, a $CO_2$-rich stream and a $CO_2$-lean stream split from the gas stream. The inert ethane is subsequently removed from the $CO_2$-rich stream during a purge. The recycle gas stream and $CO_2$ lean stream are then combined and supplied to the heat exchanger's feed.

The purge is a device that uses a vacuum to remove the inert ethane from the $CO_2$ rich stream. The vacuum lowers the pressure of the stream, which causes the ethane to vaporize. The vaporized ethane is then removed from the stream by a condenser.

### 4.1.7. Distillation Column:

Unconverted acetic acid (AA) is separated from water and vinyl acetate (VA) in a distillation column. The VA and water phases can separate because the condensed overhead product is separated in a decanter. The organic and aqueous compounds that are left behind are then sent to another distillation stage for additional purification.

The bottom distillation column product, acetic acid, is recycled back to the vaporizer together with fresh acetic acid. A part of this bottom stream is used as the wash acid in the absorber after it has cooled.

### 4.1.8. VAM Recovery:

The VAM recovery process consists of three steps:

**Absorption**: The first step is to absorb the VAM and other liquids in acetic acid. This is done in an absorber, which is a device that uses a liquid to absorb a gas. In this case, the acetic acid absorbs the VAM and other liquids from the gas stream.

**Fractional distillation**: The second step is to separate the VAM from the acetic acid by fractional distillation. This is done in a distillation column, which is a device that separates liquids based on their boiling points. The VAM has a lower boiling point than the acetic acid, so it will vaporize first and be collected at the top of the column.

**Decantation**: The third step is to separate the VAM from the water by decantation. This is done by pouring the mixture of VAM and water into a decanter, which is a device that allows the two liquids to separate based on their densities. The VAM will be on top of the water, so it can be easily removed.

## 4.2. Hazards:

### 4.2.1. Flammability:

Vinyl acetate monomer (VAM) is a flammable liquid. It has a flash point below 37°C (100°F), which means that it can vaporize and form an ignitable mixture with air at room temperature. VAM vapors are heavier than air, so they will sink to the ground and travel along the floor. This means that a VAM vapor can travel a long distance to a source of ignition, such as a flame or electric spark, and ignite **[10]**.

### 4.2.2. Reactivity:

Vinyl acetate monomer (VAM) is a reactive molecule. It can polymerize, or form long chains, if it is not inhibited or if it is not handled and stored properly. VAM is typically inhibited with a polymerization inhibitor, such as hydroquinone (HQ). When stored under the recommended conditions, VAM is stable and will not polymerize. VAM can also hydrolyze in water. This reaction is not considered dangerous because it is usually not violent. When VAM and water are combined, the polymerization and hydrolysis reactions do not occur. This is because the water molecules inhibit the polymerization reaction and the hydrolysis reaction is slowed down by the water. It is important to be aware of the hazards associated with VAM polymerization and hydrolysis and to take the necessary safety precautions to prevent these reactions from occurring**[11]**.

### 4.2.3. Health Effects:

As with all chemical compounds, the quantity and duration of exposure have a substantial impact on the health impacts associated with VAM exposure. Since VAM irritates the upper respiratory tract, skin, and eyes, contact with vapors and liquids should be avoided. The threshold for odor perception, according to reports, is at 0.5 ppm. VAM has the potential to irritate, expand, and cause eye redness and edema. VAM vapors have been found to be intolerably irritating to the eyes at 21 ppm, but not at 5 to 10 ppm. Skin sensitivity is not thought to be brought on by VAM. Laboratory animals have shown that water consumption over a lifetime or exposure to VAM can cause cancer. Tumors appeared in the tissues that had direct contact with VAM, such as the mouth, esophagus, and stomach if eaten or the nose and upper respiratory tract if inhaled. The enzymatic conversion of VAM by tissue carboxylesterases to acetaldehyde and acetic acid is regarded to be a key event in the threshold-based tumor process. Acetaldehyde is a byproduct of food metabolism and is present in low concentrations in both the environment and the body. If threshold exposure values for VAM are exceeded, acetaldehyde may accumulate above background levels. Acetaldehyde, which is also mutagenic, is thought to mediate the genotoxicity caused by VAM. **[12].**

### 4.2.4. Environmental Effects:

If released into the environment, VAM will divide up into the compartment of that environment. If discharged into the air, VAM has a tendency to remain there where it is quickly broken down by photochemical processes. It has been determined that the VAM atmospheric half-life is 0.6 days. Following discharges of VAM to soil or water, some volatilization may take place. When released into water, VAM divides mostly there and goes through hydrolysis. At pH 7 and 25°C (77°F), the hydrolytic half-life of VAM is thought to be around 7 days. VAM hydrolysis results in the hydrolysis of acetic acid and acetaldehyde. In general, hydrolysis intensifies in neutral environments. It is not anticipated that VAM will adsorb heavily to sediments or soils. VAM is considered to be toxic in aquatic environment **[13]**.

# Chapter 5

# Material Balance

# Material Balance

## Basis:

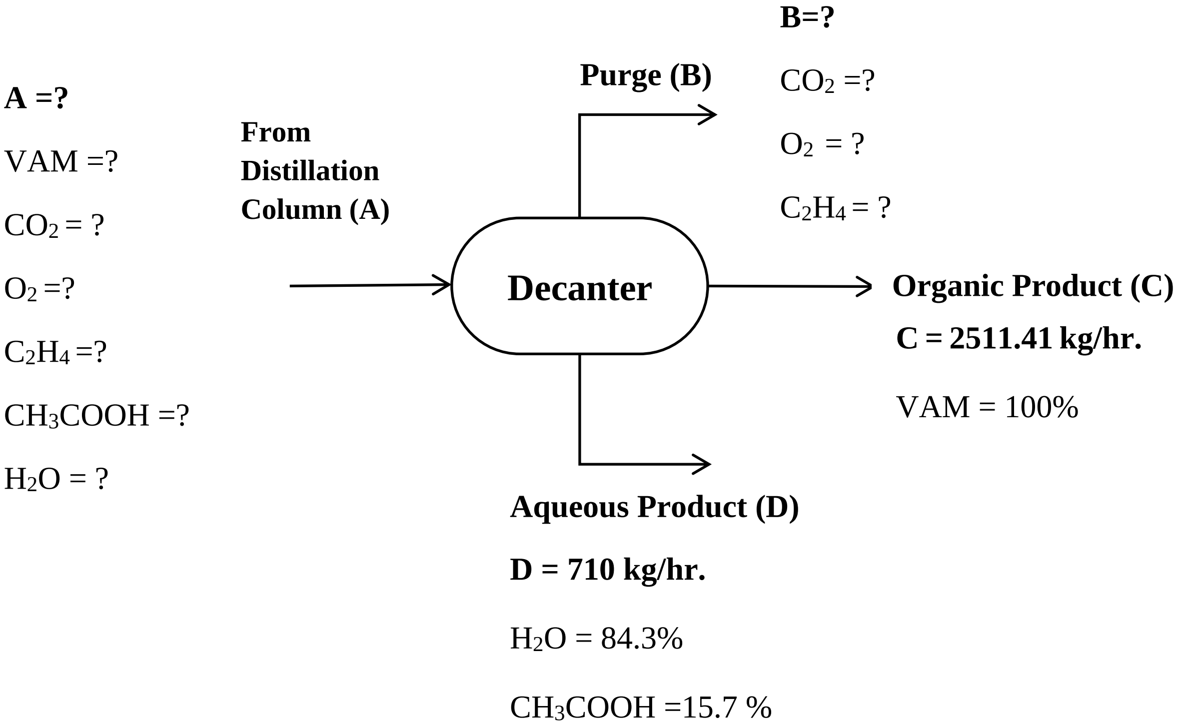
Production capacity of plant = 22,000tons/yr.

| | | | |
|---|---|---|---|
| 22,000 ton | 1 yr. | 1 day | 1000 kg |
| Yr. | 365 days | 24 hr. | 1 ton |

= 2511.41 kg/hr.

We gather the data and made assumption for this material balance from literature survey.

## 5.1. Decanter:



## For Outlet C (Organic Product):

C Stream = 2511.41 kg/hr.

## For Outlet D (Aqueous Product):

$H_2O$ = (84.3/100) *710 = 598.5 kg/hr.

$CH_3COOH$ = (15.7/100) *710 = 111.4 kg/hr.

D Stream = 710 kg/hr.[1]

## For Outlet B (Purge):

By literature survey we get the out flow rate of Decanter[1] as shown below;

B Stream = 430 kg/hr.

$CO_2$ = 43.6%

$O_2$ = 0.52%

$C_2H_4$ = 55.8%

## Overall, Balance:

**A = B + C + D**

A= 430 + 2511.41 + 710

B = 430 + 2511.41 + 710

A Stream = 3651.41 kg/hr.

## For Inlet A (From Distillation Column):

## Component (VAM):

A (%VAM) = C (%VAM)

3651.41 (%VAM) = 2511.41 (100)

**VAM** = 251141/3651.41= **68.77%**

## Component ($CO_2$):

A (%$CO_2$) = B (%$CO_2$)

3651.41(%$CO_2$) = 430 (43.6)

$CO_2$ = 5.13%

## Component ($O_2$):

A (%$O_2$) = B %($O_2$)

3651.41(%$O_2$) = 430(0.52)

($O_2$) = 0.061%

## Component ($C_2H_4$):

A (%$C_2H_4$) = B (%$C_2H_4$)

3651.41(%$C_2H_4$) = 430(55.8)

$C_2H_4$ = 6.57%

## Component ($CH_3COOH$):

A (%$CH_3COOH$) = D (%$CH_3COOH$)

3651.41 (%$CH_3COOH$) = 710 (15.7)

$CH_3COOH$ = 3.05%

## Component ($H_2O$):

A (%$H_2O$) = D (%$H_2O$)

3651.41 (%$H_2O$) = 710 (84.3)

$H_2O$ = 16.39%

## Result:

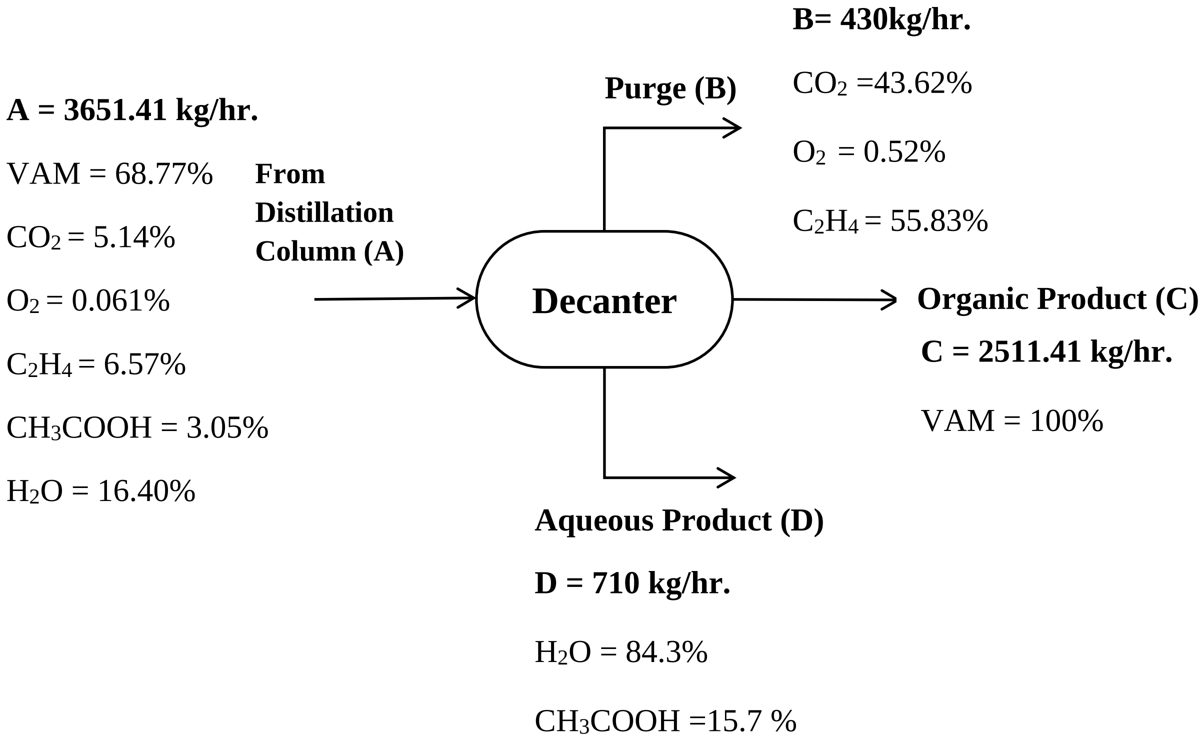
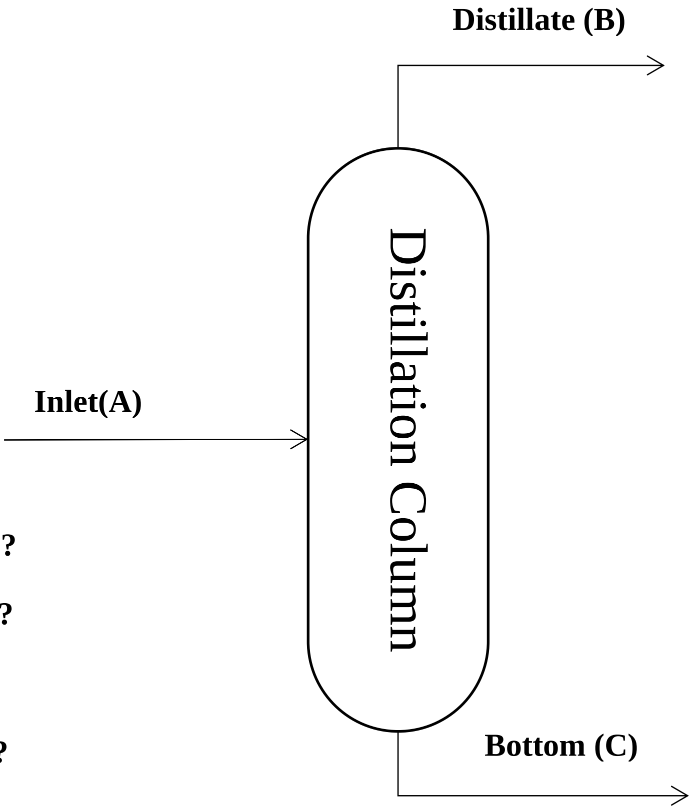


**Table 5:** Material Balance Across Decanter

| Components | Inlet (A) kg/hr. | Organic Phase (C) kg/hr. | Aqueous Phase (D) kg/hr. | Purge Stream (B) kg/hr. |
|---|---|---|---|---|
| **VAM** | 2511.07 | 2511.41 | 0 | 0 |
| **Carbon Dioxide** | 187.682474 | 0 | 0 | 187.48 |
| **Oxygen** | 2.2275987 | 0 | 0 | 2.236 |
| **Water** | 598.83124 | 0 | 598.53 | 0 |
| **Acetic Acid** | 111.3623 | 0 | 111.47 | 0 |
| **Ethylene** | 239.897637 | 0 | 0 | 239.94 |
| **Sum** | 3651.41 | 2511.41 | 710 | 430 |

## 5.2. Distillation Column:



**B = 3651.41 kg/hr.**

VAM = 68.77%

$CO_2$ = 5.14%

$O_2$ = 0.061%

$C_2H_4$ = 6.57%

$CH_3COOH$ = 3.05%

$H_2O$ = 16.40%

**A =?**

VAM **=?**

$CO_2$ **= ?**

$O_2$ **=?**

$C_2H_4$ **=?**

$CH_3COOH$ **=?**

$H_2O$ **= ?**

C=?

$H_2O$ =?

$CH_3COOH$ =?

### For Outlet C (Bottom):

### Assumptions:

- Acetic Acid = 99 Percent in Bottom and <u>C = 11053.47963kg/hr.</u>

### Overall, Balance:

**Inlet = Distillate + Bottom**

**A=B +C**

A = 3651.41 + 11053.47963

A = <u>14704.88</u>

## For Inlet A (Inlet):

## Assumptions:

- VAM = 100 Percent in Inlet

## Component (VAM):

A (%VAM) = B (%VAM)

14704.88 (%VAM) = 3651.41 (68.77)

**VAM** = 251141/3651.41= **17.07%**

## Component ($CO_2$):

A (% $CO_2$) = B (% $CO_2$)

14704.88 (% $CO_2$) = 3651.41 (5.14)

**$CO_2$ = 1.2763%**

## Component ($O_2$):

A (% $O_2$) = %( $O_2$)

14704.88 (% $O_2$) = 3651.41 (0.061)

($O_2$) = 0.0151%

## Component ($C_2H_4$):

A (% $C_2H_4$) = B (% $C_2H_4$)

14704.88 (% $C_2H_4$) = 3651.41 (6.57)

$C_2H_4$ = 1.6314 %

## Component ($CH_3COOH$):

## Assumptions:

Acetic Acid **= 99 Percent** in Bottom

A (%$CH_3COOH$) = B (%$CH_3COOH$)

14704.88 (%$CH_3COOH$) = 3651.41 (3.05)

$CH_3COOH$ = 0.7573 *99%

$CH_3COOH$ = 74.97%

## Component ($H_2O$):

A (%$H_2O$) = B (%$H_2O$)

14704.88 (%$H_2O$) = 3651.41 (16.40)

$H_2O$ = 4.07233%

## For Outlet C (Bottom):

## Component ($H_2O$):

A (%$H_2O$) = B (%$H_2O$) + C (%$H_2O$)

14704.88 (4.07) = 59883.124 + 11053.47963 (%$H_2O$)

59848.8616 -59883.124 = 11053.47963 (%$H_2O$)

$H_2O$ = 0.00309%

## Component ($CH_3COOH$):

A (%$CH_3COOH$) = B(%$CH_3COOH$) + C (%$CH_3COOH$)

14704.88 (74.97) = 11136.80+11053.47963 (%$CH_3COOH$)

$CH_3COOH$ = 99.6 %

## Results:

**A = 14704.88963 kg/hr.**

VAM = 17.07%

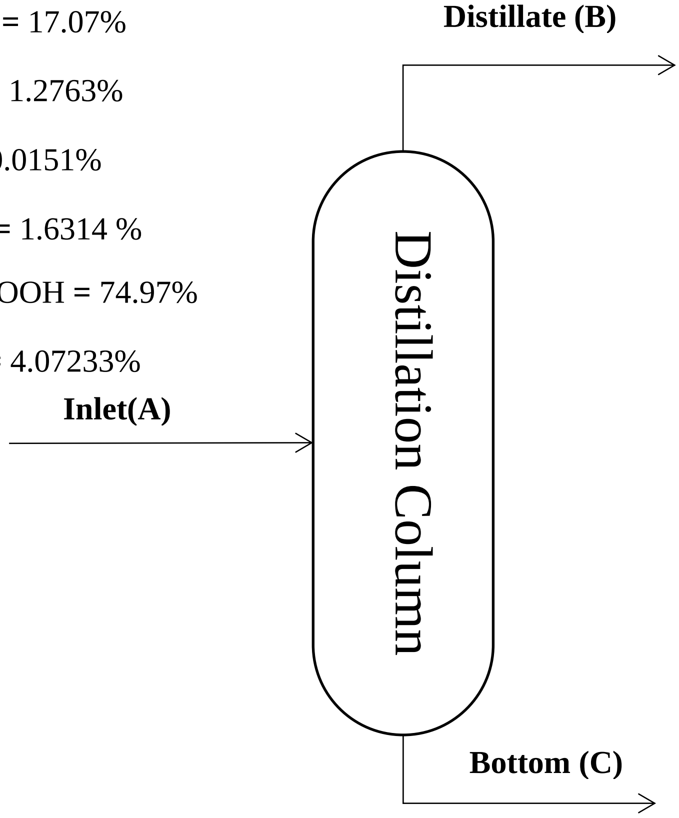
$CO_2$ = 1.2763%

$O_2$ = 0.0151%

$C_2H_4$ = 1.6314 %

$CH_3COOH$ = 74.97%

$H_2O$ = 4.07233%



**B = 3651.41 kg/hr.**

VAM = 68.77%

$CO_2$ = 5.14%

$O_2$ = 0.061%

$C_2H_4$ = 6.57%

$CH_3COOH$ = 3.05%

$H_2O$ = 16.40%

**C = 11053.47963kg/hr.**

$H_2O$ = 0.00309%

$CH_3COOH$ = 99.6 %

**Table 6:** Material Balance across Distillation Column

| Components | Inlet (A) kg/hr. | In Distillate (B) kg/hr. | In Bottom (C) kg/hr. |
|---|---|---|---|
| **VAM** | 2510.12 | 2511.07 | 0 |
| **Carbon Dioxide** | 187.68 | 187.682474 | 0 |
| **Oxygen** | 2.2273 | 2.2275987 | 0 |
| **Water** | 598.83124 | 598.83124 | 0.34155 |
| **Acetic Acid** | 11024.24 | 111.3623 | 11009.26571 |
| **Ethylene** | 239.8954 | 239.897637 | 0 |
| **Sum** | **14704.88963** | **3651.41** | **11053.47963** |

## 5.3. Mixer/Storage Tank:

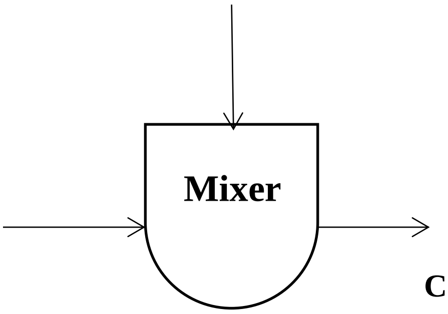
**B =?**

VAM =?

$CH_3COOH$ =?

$H_2O$ = ?

**From Absorber (B)**



**From Flash Separator (A)**

**A =?**

VAM =?

$CO_2$ =?

$O_2$ =?

$C_2H_4$ =?

$CH_3COOH$ = ?

$H_2O$ = ?

**After Mixing(C)**

**C = 14704.88963 kg/hr.**

VAM = 17.07%

$CO_2$ = 1.2763%

$O_2$ = 0.0151%

$C_2H_4$ = 1.6314 %

$CH_3COOH$ = 74.97%

$H_2O$ = 4.07233%

## For Inlet B (Absorber):

## Assumptions:

- 9.15% VAM obtain from Absorber

= (% of VAM in Absorber/100) *(VAM flow rate After Mixing)

= (9.15/100) *2510.12

VAM = 229.6756 kg/hr.

- 2.212% $H_2O$ obtain from Absorber

= (% of $H_2O$ in Absorber/100) *($H_2O$ flow rate After Mixing)

= (2.21/100) *598.83124

$H_2O$ = 13.2341kg/hr.

- 53.59% $CH_3COOH$ obtain from Absorber

= (% of $CH_3COOH$ in Absorber/100) *($CH_3COOH$ flow rate After Mixing)

= (53.59/100) *11024.24

$CH_3COOH$ = 5908.70 kg/hr.

**B =** $CH_3COOH$ + $H_2O$ + VAM

**B =** 5908.70 + 13.2341 + 229.6756

**B = 6151.6130 kg/hr.**

**VAM in A = (**229.6756/6151.6130) *100

**VAM in A** = 3.733%

**$H_2O$ in A = (**13.2341/6151.6130) *100

**$H_2O$ in A** = 0.2151%

**$CH_3COOH$ in A = (**5908.70/6151.6130) *100

**$CH_3COOH$ in A** = 96.0512%

## Overall, Balance:

**Separator + Absorber = After Mixing**

**A + B = C**

**A = -B + C**

A = - 6151.6130 + 14704.88963

**A = 8553.27663 kg/hr.**

## For Separator A (Inlet):

## Component (VAM):

A (%VAM) + B (%VAM) = C (%VAM)

8553.27663 (%VAM) = 14704.88963*(17.07) - 6151.6130*(3.733)

**VAM = 26.66%**

## Component ($CO_2$):

A (%$CO_2$) + B (%$CO_2$) = C (%$CO_2$)

8553.27663 (%$CO_2$) = 14704.88963* (1.2763) - 6151.6130*(0)

**$CO_2$ = 2.1942%**

## Component ($O_2$):

A (%$O_2$) + B (%$O_2$) = C (%$O_2$)

8553.27663 (%$O_2$) = 14704.88963* (0.0151) - 6151.6130*(0)

**$O_2$ = 0.02596009%**

## Component ($C_2H_4$):

A (%$C_2H_4$) + B (%$C_2H_4$) = C (%$C_2H_4$)

8553.27663 (%$C_2H_4$) = 14704.88963* (1.6314) - 6151.6130*(0)

**%$C_2H_4$ = 2.804721276%**

## Component ($CH_3COOH$):

A (%$C_2H_4$) + B (%$CH_3COOH$) = C (%$CH_3COOH$)

8553.27663 (%$CH_3COOH$) = 14704.88963* (74.97) - 6151.6130*(96.0512)

**$CH_3COOH$ = 59.8081%**

## Component ($H_2O$):

A (%$H_2O$) + B (%$H_2O$) = C (%$H_2O$)

8553.27663 (%$H_2O$) = (14704.88963*4.07233) - (6151.6130*0.2151)

**$H_2O$ = 6.8464%**

## Results:

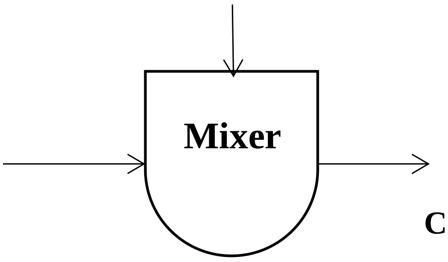
**B = 6151.6130 kg/hr.**

VAM = 3.733%

$CH_3COOH$ = 96.0512%

$H_2O$ = 0.2151%

**From Absorber (B)**



**From Flash Separator (A)**

**A = 8553.27663 kg/hr.**

VAM = 26.66%

$CO_2$ = 2.1942%

$O_2$ = 0.02596009%

$C_2H_4$ =2.804721276%

$CH_3COOH$ = 59.8081%

$H_2O$ = 6.8464%

**After Mixing(C)**

**C = 14704.88963 kg/hr.**

VAM = 17.07%

$CO_2$ = 1.2763%

$O_2$ = 0.0151%

$C_2H_4$ = 1.6314 %

$CH_3COOH$ = 74.97%

$H_2O$ = 4.07233%

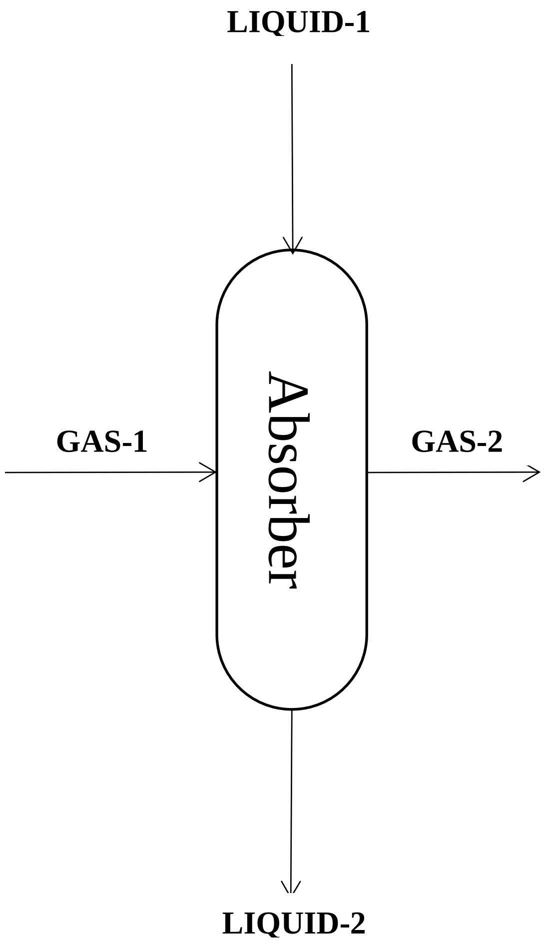
**Table 7:** Material Balance across Mixer

| Components | From Flash Separator (A) kg/hr. | From Absorber (B) kg/hr. | After Mixing (C) kg/hr. |
|---|---|---|---|
| **VAM** | 2280.30355 | 229.6756 | 2510.12 |
| **Carbon Dioxide** | 187.6759958 | 0 | 187.68 |
| **Oxygen** | 2.220438311 | 0 | 2.2273 |
| **Water** | 239.8955694 | 13.2341 | 598.83124 |
| **Acetic Acid** | 5115.55224 | 5908.70 | 11024.24 |
| **Ethylene** | 239.8955694 | 0 | 239.8954 |
| **Sum** | **8553.27663** | **6151.6130** | **14704.88963** |

## 5.4. Absorber:

**B =?**

$CH_3COOH$ =?



**A =?**

VAM =?

$CO_2$ =?

$O_2$ =?

$C_2H_4$ =?

$CH_3COOH$ =?

$H_2O$ = ?

**C =?**

$O_2$ =?

$C_2H_4$ =?

$CO_2$ = ?

**D = 6151.6130 kg/hr.**

VAM = 3.733%

$CH_3COOH$ = 96.0512%

$H_2O$ = 0.2151%

## For Inlet liquid 1 of Absorber (B):

## Assumptions:

98.77% of Acetic acid of Bottom outlet liquid stream D(L2) is present in top Inlet liquid stream B(L1)

= (98.77/100) *5908.70

**B = 5836.022 kg/hr.**

## For Outlet Gas 2 from Absorber (C):

By literature survey we get the out flow rate of Gas 2 from Absorber[1] as shown below; **C=13627.21628 kg/hr.**

## Assumptions:

**$CO_2$** = 45.10% = (45.10/100) *13627.21628 **= 6146.93 kg/hr.**

**$O_2$** = 3.27% = (3.27/100) *13627.21628 = **445.73 kg/hr.**

**$C_2H_4$** = 51.62% = (51.62/100) *13627.21628 **= 7034.54 kg/hr.**

**C = $CO_2$** + **$O_2$** + **$C_2H_4$**

**C = 6146.93** + **445.73** + **7034.54**

**<u>C = 13627.21628 kg/hr.</u>**

## Overall, Balance:

**Inlet Gas Bottom (G1) + Inlet Liquid Top(L1) = Outlet Gas Top (G2) + Outlet Liquid Bottom (L2)**

**A + B = C + D**

**A = -B + C + D**

A = -5836.022 +13627.21628 + 6151.6130

**<u>A = 13942.80728 kg/hr.</u>**

## For Absorber G1 (Inlet):

## Component (VAM):

A (%VAM) + B (%VAM) = C (%VAM) + D(%VAM)

13942.80728 (%VAM) = - 5836.022 (0) + 13627.21628 (0) + 6151.6130 (3.733)

13942.80728 (%VAM) = 6151.6130*(3.733)

**VAM = 1.64701203%**

## Component ($CO_2$):

A ($CO_2$%) + B ($CO_2$%) = C ($CO_2$%) + D ($CO_2$%)

13942.80728 ($CO_2$%) = - 5836.022 (0) + 13627.21628 (45.10) + 6151.6130 (0)

13942.80728 (%$CO_2$) = 13627.21628*(45.10)

**$CO_2$ = 44.07917587%**

## Component ($O_2$):

A (%$O_2$) + B (%$O_2$) = C (%$O_2$) + D(%$O_2$)

13942.80728 (%$O_2$) = - 5836.022 (0) + 13627.21628 (3.27) + 6151.6130 (0)

13942.80728 (%$O_2$) = 13627.21628*(3.27)

**$O_2$ = 3.195984592%**

## Component ($C_2H_4$):

A (%$C_2H_4$) + B (%$C_2H_4$) = C (%$C_2H_4$) + D(%$C_2H_4$)

13942.80728 (%$C_2H_4$) = - 5836.022 (0) + 13627.21628 (51.62) + 6151.6130 (0)

13942.80728 (%$C_2H_4$) = 13627.21628 (51.62)

**%$C_2H_4$ = 50.45159775%**

## Component ($CH_3COOH$):

A (%$CH_3COOH$) + B (%$CH_3COOH$) = C (%$CH_3COOH$) + D(%$CH_3COOH$)

13942.80728 (%$CH_3COOH$) = - 5836.022 (100) + 13627.21628 (0) + 6151.6130 (96.0512)

13942.80728 (%$CH_3COOH$) =- 5836.022 (100) + 6151.6130*(96.0512)

**$CH_3COOH$ = 0.521244427%**

## Component ($H_2O$):

A (%VAM) + B (%$H_2O$) = C (%$H_2O$) + D (%$H_2O$)

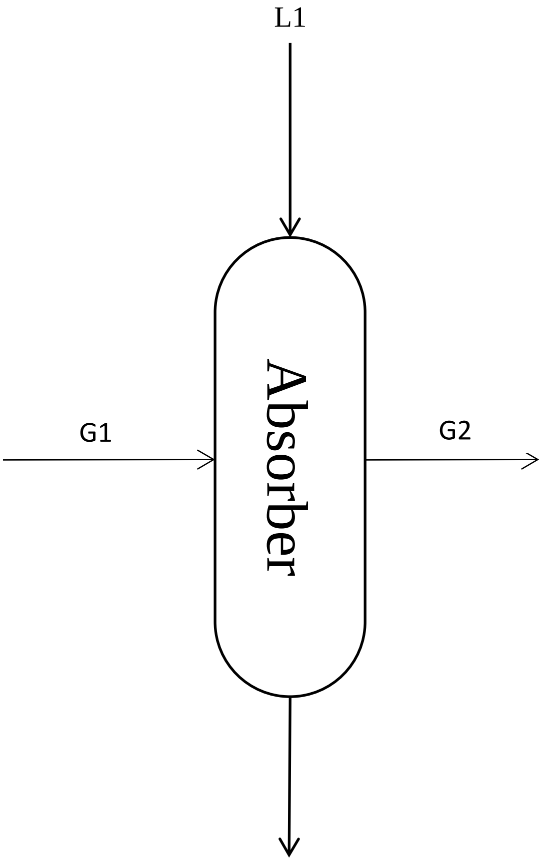
13942.80728 (%$H_2O$) = - 5836.022 (0) + 13627.21628 (0) + 6151.6130 (239.8955694)

13942.80728 (%$H_2O$) = 6151.6130*(0.2151)

**$H_2O$ = 0.094902836%**

## Results:

**B = 5836.022 kg/hr.**



**A = 13942.80728**

VAM = **1.64701203%**

$CO_2$ = **44.07917587%**

$O_2$ = **3.195984592%**

$C_2H_4$ = **50.451%**

$CH_3COOH$ = **0.521%**

$H_2O$ = **0.094902%**

**C = 13627.21 kg/hr.**

$O_2$ = 3.27%

$C_2H_4$ = 51.62%

$CO_2$ = 45.10%

**L2**

**D = 6151.6130 kg/hr.**

VAM = 3.733%

$CH_3COOH$ = 96.0512%

$H_2O$ = 0.2151%

**Table 8:** Material Balance Across Absorber

| Components | Gas-1 In (A) kg/hr. | Liquid-1 In (B) kg/hr. | Gas-2 Out (C) kg/hr. | Liquid-2 Out (D) kg/hr. |
|---|---|---|---|---|
| **VAM** | 229.639709 | 0 | 0 | 229.6756 |
| **Carbon Dioxide** | 6145.874532 | 0 | 6146.93 | 0 |
| **Oxygen** | 445.6099721 | 0 | 445.73 | 0 |
| **Water** | 13.23200296 | 0 | 0 | 13.2341 |
| **Acetic Acid** | 72.64202593 | 5836.02 | 0 | 5908.70 |
| **Ethylene** | 7034.285701 | 0 | 7034.54 | 0 |
| **Sum** | **13942.80728** | **5836.022** | **13627.21** | **6151.6130** |

## 5.5. Flash Separator/Column:

**A =?**

VAM =?

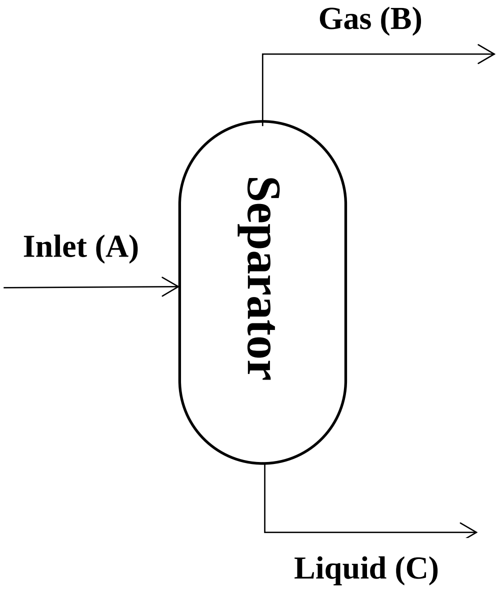
$CO_2$ = ?

$O_2$ =?

$C_2H_4$ =?

$CH_3COOH$ =**?**

$H_2O$ = ?



**B = 13942.80728 kg/hr.**

VAM = 1.64701203%

$CO_2$ = 44.07917587%

$O_2$ = 3.195984592%

$C_2H_4$ = 50.451%

$CH_3COOH$ = 0.521%

$H_2O$ = 0.094902%

**C = 8553.27663 kg/hr.**

VAM = 26.66%

$CO_2$ =2.1942%

$O_2$ = 0.02596009%

$C_2H_4$ =2.804721276%

$CH_3COOH$ = 59.8081%

$H_2O$ = 6.8464%

## Overall, Balance:

**Inlet Stream (A) = Outlet Gas Top (B) + Outlet Liquid Bottom (C)**

**A = B + C**

**A = 13942.80728 kg/hr. + 8553.27663 kg/hr.**

**<u>A = 22496.08391 kg/hr.</u>**

## For Inlet (A):

## Component (VAM):

A (%VAM) = B (%VAM) + C (%VAM)

22496.08391(%VAM) = 13627.21628 (1.64701203) + 8553.27663 (26.66)

22496.08391(%VAM) = 250474.5441

(%VAM) = (250474.5441)/ (22496.08391)

**VAM = 11.13413984%**

## Component ($CO_2$)

A (%$CO_2$) = B (%$CO_2$) + C (%$CO_2$)

22496.08391(%$CO_2$) = 13627.21628 (44.0791) + 8553.27663 (2.1942)

22496.08391(%$CO_2$) = 250474.5441

(%$CO_2$) = (619443.0287)/ (22496.08391)

**$CO_2$ = 27.5355938%**

## Component ($O_2$):

A (%$O_2$) = B (%$O_2$) + C (%$O_2$)

22496.08391(%$O_2$) = (13627.21628*3.1942) + (8553.27663*0.02596009)

22496.08391(%$O_2$) = 43750.09807

(%$O_2$) = (43750.09807)/ (22496.08391)

**$O_2$ = 1.94478729%**

## Component ($C_2H_4$):

A (%VAM) = B (%$C_2H_4$) + C (%$C_2H_4$ )

22496.08391(%$C_2H_4$) = (13627.21628*50.451) + (8553.27663*2.804721276)

22496.08391(%$C_2H_4$) = 711496.2455

(%$C_2H_4$ ) = (250474.5441)/ (22496.08391)

**%$C_2H_4$ = 31.62756008%**

### Component ($CH_3COOH$):

A (%$CH_3COOH$)  = B (%$CH_3COOH$) + C (%$CH_3COOH$)

22496.08391(%$CH_3COOH$) = (13627.21628 *0.521) + (8553.27663 *59.8081)

22496.08391(%$CH_3COOH$) = 518655.0037

(%$CH_3COOH$) = (250474.5441)/ (22496.08391)

**$CH_3COOH$ = 23.05534624%**

### Component ($H_2O$):

A (%$H_2O$) = B (%$H_2O$) + C (%$H_2O$)

22496.08391(%$H_2O$) = (13627.21628 *0.094902) + (8553.27663 *6.8464)

22496.08391(%$H_2O$) = 59852.4032

(%$H_2O$) = (59852.4032)/ (22496.08391)

**$H_2O$ = 2.660569877%**

## Result:

**A = 22496.08391 kg/hr.**

VAM = **11.134139%**

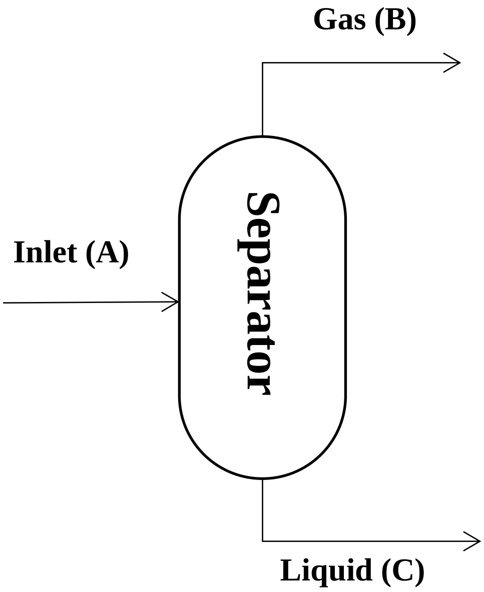
$CO_2$ = **27.5355938%**

$O_2$ = **1.94478729%**

$C_2H_4$ = **31.6275600%**

$CH_3COOH$ = **23.055%**

$H_2O$ = **2.660569877%**



**B = 13942.80728 kg/hr.**

VAM = 1.64701203%

$CO_2$ = 44.07917587%

$O_2$ = 3.195984592%

$C_2H_4$ = 50.451%

$CH_3COOH$ = 0.521%

$H_2O$ = 0.094902%

**C = 8553.27663 kg/hr.**

VAM = 26.66%

$CO_2$ =2.1942%

$O_2$ = 0.02596009%

$C_2H_4$ =2.804721276%

$CH_3COOH$ = 59.8081%

$H_2O$ = 6.8464%

**Table 9:** Material Balance Across Flash Vessel

| Components | Inlet (A) kg/hr. | Gas (B) kg/hr. | Liquid (C) kg/hr. |
|---|---|---|---|
| **VAM** | 2504.745252 | 229.639709 | 2280.30355 |
| **Carbon Dioxide** | 6394.430286 | 6145.874532 | 187.6759958 |
| **Oxygen** | 447.5009806 | 445.6099721 | 2.220438311 |
| **Water** | 598.524032 | 13.23200296 | 239.8955694 |
| **Acetic Acid** | 5186.472145 | 72.64202593 | 5115.55224 |
| **Ethylene** | 7114.962436 | 7034.285701 | 239.8955694 |
| **Sum** | **22496.08391** | **13942.80728** | **8553.27663** |

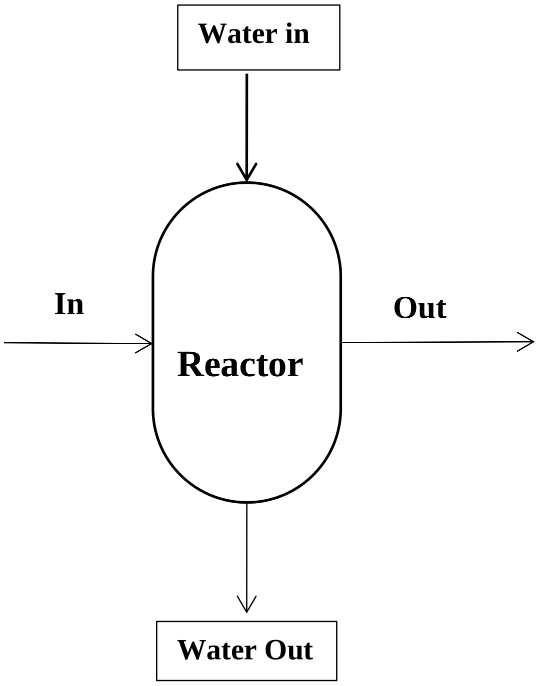
## 5.6. Multi Tubular Reactor:

**A=22496.08391 kg/hr.**

$CO_2$ = ?

$O_2$ =?

$C_2H_4$ =?



**B = 22496.08391 kg/hr.**

VAM = **11.134139%**

$CO_2$ = **27.5355938%**

$O_2$ = **1.94478729%**

$C_2H_4$ = **31.6275600%**

$CH_3COOH$ = **23.055%**

$H_2O$ = **2.660569877%**

## Assumptions:

- Steady state process
- Argon and Methane are inert

## Reactions:

**Primary reaction:**

$$C_2H_4 + CH_3COOH + 0.5O_2 \xrightarrow{Pd} C_2H_3OOCCH_3 + H_2O$$

**Secondary reaction:**

$$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$$

## Conversions:

Acetic acid = 25%

Ethylene = 10-11%

Oxygen = 60%

**Table 10:** Flow rates of outlet stream of Reactor

| Components | Outlet (B) kg/hr | Molar Mass g/mol | Outlet (B) Kmole/hr. | Mole fraction |
|---|---|---|---|---|
| **VAM** | 2504.745252 | 86.09 | 29.09449706 | 0.051799036 |
| **Carbon Dioxide** | 6394.430286 | 44 | 145.327961 | 0.258737875 |
| **Oxygen** | 447.5009806 | 32 | 13.98440564 | 0.024897448 |
| **Water** | 598.524032 | 18.01 | 33.25133511 | 0.059199756 |
| **Acetic Acid** | 5186.472145 | 60.05 | 86.36922806 | 0.15376938 |
| **Ethylene** | 7114.962436 | 28.05 | 253.6528498 | 0.451596505 |
| **Sum** | **22496.08391** | | **561.6802767** | **1** |

## For First Reaction:

$\mathbf{CH_3COOH : C_2H_4 : O_2 : C_2H_3OOCCH_3 : H_2O}$

1 : 1 : 0.5 : 1 : 1

Coefficient x Molar Mass of Components

60.053:28.054: 0.5*32:86.09: 18.015

60.053: 28.054 : 16 : 86.09 : 18.015

$$\frac{60.053}{86.09}:\frac{28.054}{86.09}:\frac{16}{86.09}:\frac{86.09}{86.09}:\frac{18.01}{86.09}$$

0.6975606923 : 0.3258682774 : 0.1858520153 : 1 : 0.2091996748

The amount of Acetic Acid outlet is 2504.745252 kg

$$0.6975606923 \text{ x } 2504.745252 : 0.3258682774\, x\, 2504.745252 : 0.1858520153\, x\, 2504.745252 :$$

$$1\ x\ 2504.745252 : 0.2091996748 \text{ x } 2504.745252$$

1747.211832 : 816.2170206 : 465.5119529 : 2504.745252 : 523.9918922

Only the first reaction uses acetic acid, hence the remaining amounts of acetic acid are now present in the product is:

Acetic acid consumed = 1747.211832

Acetic Acid conversion is 25% then

**Acetic acid inlet** = $\frac{1747.211832}{0.25}$ = 6988.84 **kg/hr.**

**Prove:**

Acetic acid remaining = total – consumed

Outlet = Inlet - consumed

Outlet = 6988.84 - 1747.211832

Outlet = 5186.472145 **kg/hr.**

The quantity of ethylene used in the first reaction = 816.2170206

Ethylene conversion is 10% then

Ethylene Inlet = $\frac{816.2170206}{0.11}$ = 7420.154545 **kg/hr.**

The quantity of oxygen used in the first reaction = 465.5119529

Oxygen conversion is 60% then

Oxygen Inlet = $\frac{465.5119529}{0.60}$ = 775.8532088 **kg/hr.**

The amount of Water consumed in 1st reaction

Water consumed = 523.9918922 kg

VAM remaining = total – consumed

VAM remaining = 2504.745252 - 2504.745252

**Acetic acid remaining = 0 kg/hr.**

## 2nd Reaction:

**$O_2 : C_2H_4 : CO_2 : H_2O$**

3 : 1 : 2 : 2

3* 32 : 1* 28.054: 2*44.01 : 2* 18.015

96 : 28.054 : 88.02 : 36.03

$$\frac{96}{36.03} : \frac{28.054}{36.03} : \frac{88.02}{36.03} : \frac{36.03}{36.03}$$

2.66444: 0.7786289: 2.4429641: 1

598.524032 x 2.66444 :598.524032 x 0.7786289: 598.524032 x 2.4429641

: 598.524032 x 1

1594.7313: 466.0281: 1462.172723: 598.524032

**$CO_2$ produced = 1462.172723 kg/hr.**

$CO_2$ in product = In Feed + Produced

6394.430286 - 1462.172723 = In Feed

4932.258286 = In Feed

Water produced for 2nd reaction = 598.524032

$H_2O$ in product = In Feed + Produced

598.524032- 598.524032 = In Feed

**Water in Feed = 0 kg/hr.**

## Results:

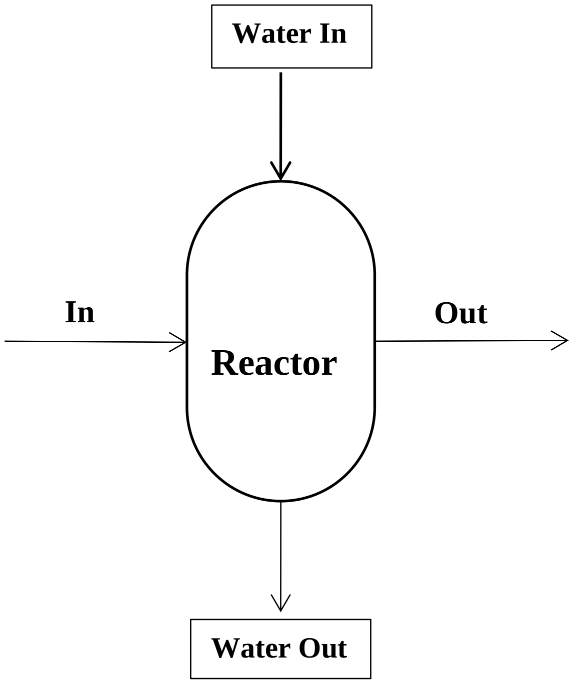
**A=22496.08391 kg/hr.**

$CO_2$ = 27.579702%

$O_2$ = 4.983065032

$C_2H_4$ =35.469%

$CH_3COOH$ = 30.830%



**B = 22496.08391 kg/hr.**

VAM = **11.134139%**

$CO_2$ = **27.5355938%**

$O_2$ = **1.94478729%**

$C_2H_4$ = **31.6275600%**

$CH_3COOH$ = **23.055%**

$H_2O$ = **2.660569877%**

**Table 11:** Material Balance Across Reactor

| Components | Inlet (A) kg/hr. | Outlet (B) kg/hr. |
|---|---|---|
| **VAM** | 0 | 2504.745252 |
| **Carbon Dioxide** | 6204.353072 | 6394.430286 |
| **Oxygen** | 1120.994491 | 447.5009806 |
| **Water** | 0 | 598.524032 |
| **Acetic Acid** | 6935.676053 | 5186.472145 |
| **Ethylene** | 7979.350424 | 7114.962436 |
| **Sum** | 22496.08391 | 22496.08391 |

# Chapter 6

# Energy Balance

**For Gas Stream:**

The correlation for heat capacity of gas is a series expansion in temperature.

$$\mathbf{Cp = a + bT + cT^{2} + dT^{3} + eT^{4}}$$

(Chemical Properties Handbook, Carl L. Yaws)

Here a, b, c, d, e is regression coefficients for chemical compound

**Table 12:** Heat capacity coefficients for Gases

| **Components** | **Heat capacity coefficients for Gases** | | | | |
|---|---|---|---|---|---|
| | **a** | **b** | **c** | **D** | **e** |
| **Acetic acid** | 34.85 | 0.037626 | 0.00028311 | -3.067E-07 | 9.2646E-11 |
| **Water** | 33.933 | -0.0084186 | 0.000029906 | -1.7825E-08 | 3.6934E-12 |
| **Oxygen** | 29.526 | -0.0088999 | 0.000038083 | -3.2629E-08 | 8.8607E-12 |
| **VAM** | 27.664 | 0.23366 | 0.000062106 | -1.6972E-07 | 5.7917E-11 |
| **Ethylene** | 32.083 | -0.014831 | 0.00024774 | -2.3766E-07 | 6.8724E-11 |
| **Carbon Dioxide** | 27.437 | 0.042315 | -0.000019555 | 3.9968E-09 | -2.9872E-13 |

## 6.1. Multi Tubular Reactor

## Reactions:

**Primary reaction:**

$$C_2H_4 + CH_3COOH + 0.5O_2 \xrightarrow{Pd} C_2H_3OOCCH_3 + H_2O$$

**Secondary reaction:**

$$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$$

<u>**Inlet Side:**</u>

A series expansion in temperature serves as the correlation for the heat capacity of gases.

$$Cp = a + bT + cT^2 + dT^3 + eT^4$$

Inlet Temperature = 147.4 C

**Table 13:** Energy Balance across reactor Inlet Side

| **Components** | **m** (kmol/hr.) | **Cp** (J/mole) | **ΔT** ($T_2-T_1$) | **Q** (kJ/hr.) |
|---|---|---|---|---|
| **VAM** | 0 | 27,699 | 11.5 | 0 |
| **Carbon Dioxide** | 141.0080244 | 33 | 11.5 | 53513 |
| **Oxygen** | 35.03107784 | 29 | 11.5 | 11683 |
| **Water** | 0 | 33 | 11.5 | 0 |
| **Acetic Acid** | 115.4983523 | 46 | 11.5 | 61099 |
| **Ethylene** | 284.4688208 | 35 | 11.5 | 114499 |
| **Sum** | **576.0062753** | | | **240,793** |

**<u>Outlet Side:</u>**

The correlation for heat capacity of gas is a series expansion in temperature.

$$Cp = a + bT + cT^2 + dT^3 + eT^4$$

Outlet Temperature = 158.9 C

**Table 14:** Energy Balance across reactor Outlet Side

| **Components** | **m** (kmol/hr.) | **Cp** (J/mole) | **ΔT** ($T_2-T_1$) | **Q** (kJ/hr.) |
|---|---|---|---|---|
| **VAM** | 29.09449706 | 27,702 | 11.5 | 0 |
| **Carbon Dioxide** | 145.327961 | 34 | 11.5 | 53513 |
| **Oxygen** | 13.98440564 | 29 | 11.5 | 11683 |

| | | | | |
|---|---|---|---|---|
| **Water** | 33.25133511 | 33 | 11.5 | 0 |
| **Acetic Acid** | 86.36922806 | 47 | 11.5 | 61099 |
| **Ethylene** | 253.6528498 | 35 | 11.5 | 114499 |
| **Sum** | 561.6802767 | | | 240,793 |

**Average Specific Heat**

| Inlet | Outlet |
|---|---|
| **KJ/kmol. K** | **KJ/kmol. K** |
| 53.45 | 54.7 |

$Q = ncp\Delta T$

**For Inlet**

$Q_{in} = n_{in} Cp_{in} \Delta T_{in}$

$Q_{in} = 581.5*53.45*125$

**$Q_{in} = 3885146.875$ (J/hr.)**

**For Outlet**

$Qout = n_{out} Cp_{out} \Delta T_{out}$

$Qout = 566.9625*54.7*125$

**$Qout = 3876606.094$ (J/hr.)**

**Q In = Q Out**

**Change in Enthalpy ΔH**

ΔHr1 at $25^0$ C= **-5123015 kJ/hr.**

ΔHr2 at $25^0$ C = **-2820430 kJ/hr.**

ΔHr1 at $148^0$C = (nCp ΔT) reactants + ΔHr1 at 25°C + (nCp ΔT) products

**= -5151598 kJ/hr.**

ΔHr2 at 148°C = (nCp ΔT) reactants + ΔHr2 at 25°C + (nCp ΔT) products

**= -2731842 kJ/hr.**

$\Delta$Hr. = -5151598 - 2731842

**= -7883440 KJ/hr.**

**Q = Qin - Qout + $\Delta$Hr.**

= 3885146 – 3876606 - 7883440

= -7874900 KJ/hr.

**= -2187.47 KW**

For water flow rate

$Q = nCp\Delta\mathrm{T}$

$$m = \frac{Q}{Cp\Delta\mathrm{T}}$$

m= 0.65 kmol/ sec = 11.7 kg/

sec

**= 4.212 ton/hr.**

## 6.2. Heat Exchanger:

| Stream | Cp $_{avg}$ (J/kg °C) | m(kg/hr.) |
|---|---|---|
| Hot side Stream(gas) | 1177.600 | 22399.11 |
| Cold side Stream(gas) | 1629.58 | 13627.21 |

**Heat released from Hot stream:**

**Qh = mCp$\Delta$T**

$Q_h$ = 22402.8319*1177.600*-50

$Q_h$ = -1321059.7026 kJ/hr.

$Q_h$ = -366961.0285 W

**Heat absorbed by cold stream:**

**Qc = mCp$\Delta$T**

$Q_C$ =13629.538998*1.3415 *58.6

$Q_C$ = 1321059.7026 kJ/hr.

$Q_C$ = 366961.0285 W

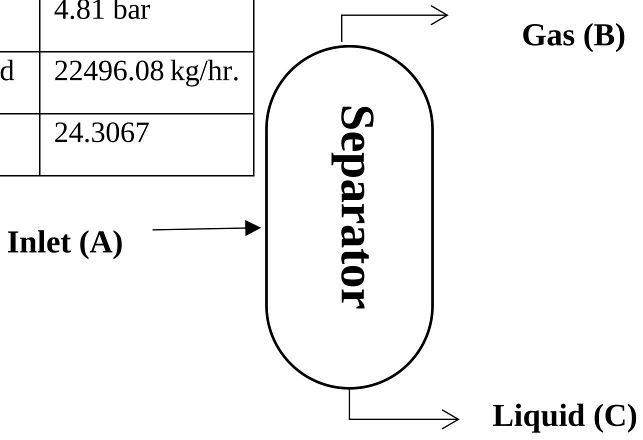
**Heat absorbed = Heat released**

1321059.7026 kJ/hr.= -1321059.7026 kJ/hr.

## 6.3. Flash Separator /Column:

| Heat Flow of Vapor Outlet | |
|---|---|
| Final Temperature | 308.5 K |
| Pressure | 4.81 bar |
| Mass Flow rate of feed | 13948.08 kg/hr. |
| Cp Average at 298K | 36.75 KJ/Kg. K |

| Heat Flow of Feed | |
|---|---|
| Final Temperature | 308.5 K |
| Pressure | 4.81 bar |
| Mass Flow rate of feed | 22496.08 kg/hr. |
| Cp Average at 298K | 24.3067 |



| Heat Flow of Liquid Outlet | |
|---|---|
| Final Temperature | 308.5 K |
| Pressure | 4.81 bar |
| Mass Flow rate of feed | 8553.27 kg/hr. |
| Cp Average at 298K | 3.77 KJ/Kg. K |

**Q = mCpΔT**

**For feed**

Q = 22496.08* 24.3066 * 9.5 **= 5194630.572 kJ/hr. = 1442.952937 KW**

**For Gaseous Phase**

Q = 13948.08* 36.7554592 *9.5 **= 4870338.967 kJ/hr. = 1352.871935KW**

**For Liquid Phase**

Q = 8553.27* 3.777764072 * 9.5 **= 306961.0368 kJ/hr. = 85.266955KW**

**Table 15:** Energy Balance Across Heat Exchangers

| HEAT FLOWS | | |
|---|---|---|
| **Feed** | **Vapor** | **Liquid** |
| 5194630.572 **KJ/hr.** | 4870338.967 **KJ/hr.** | 306961.0368 **KJ/hr.** |
| 1442.952937 **KW** | 1352.871935 **KW** | 85.266955 **KW** |

## 6.4. Absorber

### Heat Flow of Feed

| **Temperature** | 308.5 K |
|---|---|
| **Pressure** | 4.81 bar |
| **Feed Flow Rate** | 13942.8072 Kg/hr. |
| **Qin = mCpΔT** | **165835.5 kJ / kgmole** |

### Heat Flow of Dilute VAM

| **Temperature** | 308.5 K |
|---|---|
| **Pressure** | 4.81 bar |
| **Feed Flow Rate** | 6151.61 Kg/hr. |
| **Qin = mCpΔT** | **71991.69 kJ / kgmole** |

### Heat Flow of Top Gases

| **Temperature** | 308.5 K |
|---|---|
| **Pressure** | 4.81 bar |
| **Feed Flow Rate** | 13627.61 Kg/hr. |
| **Qin = mCpΔT** | **117338.9 kJ / kgmole** |

### Overall Heat Flow

**$Q_{out} = Q_{top} + Q_{bottom}$**

71991.69 + 117338.9 = 189330.59KJ/hr.

Q = Qout – Qin + ΔHr.

= 189330.59 - 13942.8072 - 316000

Q = -140612.2172 kJ / hr.

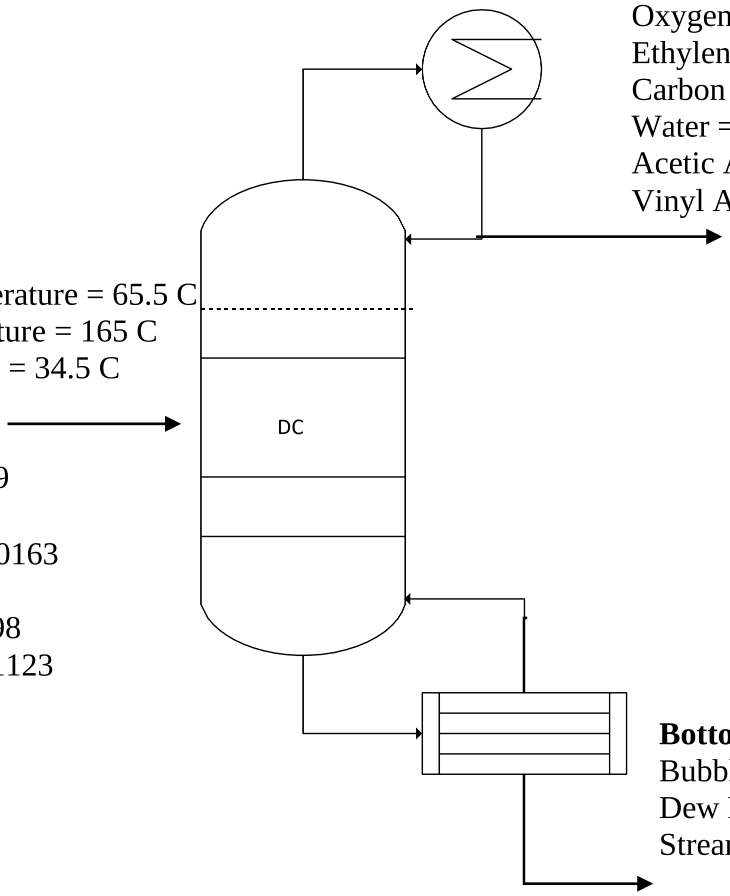
**Mass flow rate of Absorbent (Acetic Acid)**

m = Q / (Cpavg $\Delta$T) **= 23.53 kg / hr.**

## 6.5. Distillation Column:

**Top Stream:**
Bubble Point Temp = 51.5 C
Dew Point Temp = 82.5 C
Stream Temp = 75 C

**Mol. Fraction:**
Oxygen = 0.000912
Ethylene = 0.11106
Carbon dioxide = 0.0553
Water = 0.4313
Acetic Acid = 0.02411
Vinyl Acetate = 0.3772



**Feed Stream:**
Bubble Point Temperature = 65.5 C
Dew Point Temperature = 165 C
Stream Temperature = 34.5 C

**Mol. Fraction:**
Oxygen = 0.0002689
Ethylene = 0.03274
Carbon dioxide = 0.0163
Water = 0.12845
Acetic acid = 0.71098
Vinyl Acetate = 0.11123

**Bottom Stream:**
Bubble Temp = 126 C
Dew Point Temp = 127 C
Stream Temp = 129 C

**Mol. Fraction:**
Water = 0.0018
Acetic Acid = 0.998

## Feed Stream:

$$\mathbf{Cp = a + bT + cT^2 + dT^3 + eT^4 = J/\ kgmole}$$

Cp Avg = 169.5829 kJ/kmol. K

m= F= 261.355 kgmole/hr.

$$\Delta H_F = mCp\Delta T$$

$$\Delta H_F = 421052.3561 \text{ kJ/hr.} = 116.958 \text{ kW}$$

**Enthalpy of Liquid in distillate:**

$$\mathbf{Cp = a + bT + cT^2 + dT^3 + eT^4 = J/\ kgmole}$$

Cp Avg = 197.931 kJ/ kgmole. K

m= D = 77.057 kgmole/hr.

**$\Delta H_d$= mCp$\Delta$T**

$\Delta H_d$ = 762606.93 kJ/hr. = 211.835 kW

R = 0.879

L = RD = 67.73897 kgmole/hr.

V = L + D = 144.79673 kgmole/hr.

**Enthalpy of Vapors at top:**

$$\mathbf{Cp = a + bT + cT^2 + dT^3 + eT^4 = J/\ kgmole}$$

$$\text{Cp Avg} = 197.931 \text{ kJ/ kgmole. K}$$

The following formula converts the latent heat of vaporization at the boiling point of the constituents for stream conditions:

$$\mathbf{(ʎ_2/ʎ_1) = (Tr_1/Tr_2)\ \hat{}\,0.38}$$

$Tr_1$ = Reduced Bubble point of feed stream

$Tr_2$ = Reduced Dew point of Top stream

| Component | LHV kJ/mol | J/Kmol |
|---|---|---|
| **Water** | 40.65 | 40650 |

| | | |
|---|---|---|
| **Acetic Acid** | 39.82 | 39820 |
| **VAM** | 31.4 | 31400 |

$\lambda$= 29877.97 kJ/kgmole. K

$T_f$ = 338 K

$T_r$ =298 K

$m$= $V$ = 144.796 kgmole/hr.

$\Delta H_V$= m Cp $\Delta$T + m $\lambda$

$\Delta HV$ = 5759221.677 kJ/hr. = 1599.784 kW

**Enthalpy of liquid refluxed back at top:**

$\lambda_{avg}$ =317.4 kJ/ kgmole. K

$T_{f=}$ 338 K

$T_r$=298 K

m= L =67.738 kgmole/hr.

$\Delta H_L$= mCp$\Delta$T

$\Delta H_L$ = 870986.5 kJ/hr. = 241.94 kW

## Calculation of Heat Duties:

### Condenser Duty:

The energy balance before and after the condenser, which can be expressed as follows, can be used to calculate the condenser duty.

Heat Leaving = Heat Entering

Enthalpy of vapors entering the condenser equals the sum of the heat removed, the distillate's enthalpy, and the reflux stream's enthalpy.

Q = 1146.008 kW

**Water flow rate:**

Cp= 4.18 kJ / kg. K

$\Delta T$ =348 – 298= 50K

$Q= mCp\Delta T$

$m = Q/Cp\Delta T$

m = 19739.848 Kg/hr.

M= 5.483 kg/sec

**Reboiler Duty:**

A distillation column's reboilers heat output can be determined using an energy balance. The feed, distillate, bottom stream, and reboiler make up the system under study. The amount of heat entering and leaving the system is equal. The heat generated by the feed's vaporization is the heat that enters the system. The amount of heat needed to vaporize a liquid is known as the heat of vaporization. Condensation of the distillate and bottom stream vaporization generate the heat that leaves the system.

The amount of heat emitted when a vapor condenses to a liquid is known as the heat of condensation. According to the energy balance,

(Heat entering the system = Heat leaving the system) = 1932.8522 kW

**Qin = Qout**

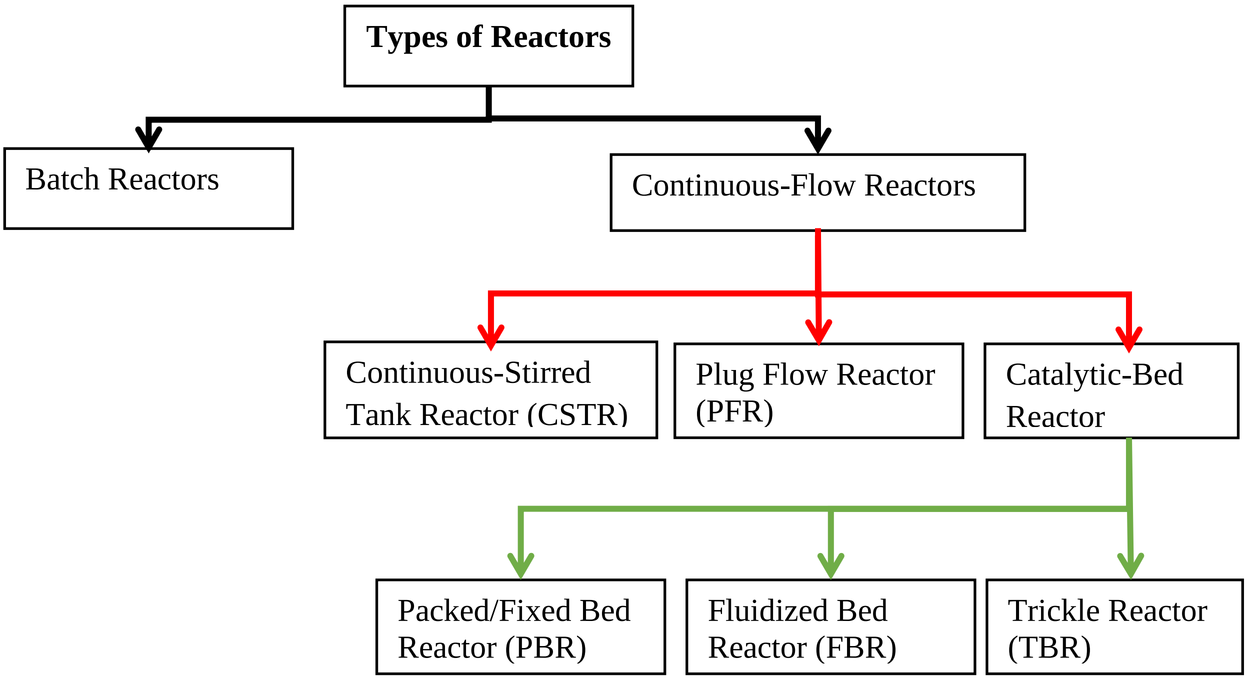
# Chapter 7

# Equipment Design

## Reactor:

The reactor is the core of the chemical plant. It is the most common unit process equipment in the industry. Reactors are vessels that are intended to contain the chemical reactions involved. The significance of reactors stems from their ability to facilitate chemical reactions in a controlled and efficient manner, which is essential to produce high-quality products. A critical aspect of a reactor is reactor design, which must consider factors such as heat and mass transfer, and reaction kinetics to guarantee that the reaction occurs efficiently and safely.

### 7.1.1. Types of Reactors:



**Other:**

- Slurry Reactor
- Segregated Tank Reactor
- Metal Gauze Reactors
- External Recycle Reactor
- Monolith Reactors
- Berty Reactors
- Carberry (Spinning Basket) Reactor
- Counter Diffusive Reactor

**Table 16:** Choice of Reactors

| Reactor Type | Advantages | Disadvantages | Area of Application |
|---|---|---|---|
| **Batch Reactor** | ▪ Suitable for small scale production.<br>▪ Suitable for long time reactions.<br>▪ Suitable for high selectivity. | ▪ Not designed for large scale production<br>▪ Closed system | ▪ Micro-Chemical Industry |
| **Continuous Stirred Tank Reactor (CSTR)** | ▪ High flexibility; increased concentration gradient.<br>▪ Between reactions, during the process, byproducts can be eliminated. | ▪ Complex and expensive as compared to tubular reactor.<br>▪ Assumed that mixing is perfect | ▪ Chemical reactions involving gas and liquids. |
| **Tubular Reactor (PFR)** | ▪ Reactants can be submerged under several circumstances.<br>▪ When compared to CSTR, it is more efficient and multitubular. | ▪ Not cost effective for small scale production | ▪ Chemical production at cryogenic and hyperthermic temperatures. |

It is not possible to assume perfect mixing because both reactions are catalytic. Also, the production size is too large for a batch reactor. As a result, the production will use a multi-tubular catalytic reactor, which is less complex and more economically feasible for VAM plants.

### 7.1.2. Design Steps:

1. Identify the desired flow rates and operating conditions
2. Choose and appropriate catalyst and particle size.
3. Choose the appropriate configuration for the reactor.
4. Evaluate the reaction rate through the analysis of experimental data.
5. Determine the catalyst's weight using the design equation for a Packed Bed Reactor.
6. Determine the volume occupied by the catalyst.
7. Determine the number of tubes required.
8. Determine the tube's diameter and length using the L/D ratio.
9. Determine the dimensions and quantity of the tubes.
10. Determine the volume of the shell surrounding the reactor.
11. Determine the reactor's diameter and length using the L/G ration
12. Assess the pressure drop within the system.
13. Choose a suitable construction material.
14. Develop an initial mechanical design for the reactor.

### 7.1.3. Reaction Equation:

- **Primary Reaction:**

$$C_2H_4 + CH_3COOH + 0.5O_2 \xrightarrow{\textbf{Pd}} C_2H_3OOCCH_3 + H_2O$$

- **Secondary Reaction:**

$$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$$

For the production of vinyl acetate, gas-phase processes are favored because they result in a better yield and are less likely to corrode. Because it reduces yield and makes it more challenging to remove reaction heat, the combustion of ethylene to carbon dioxide is a highly unfavorable secondary reaction.

The amount of heat released or absorbed when one mole of substance reacts under typical circumstances is known as the standard heat of reaction. In this instance, the conventional heats of reaction for ethylene combustion and vinyl acetate combustion are **-1322.8 Kcal/KJ per mol** and **-176.2 Kcal/KJ per mol**, respectively. When these two reactions are allowed to occur simultaneously the heat released from combustion of vinyl acetate is added to the heat released from combustion of ethylene. This results in an overall heat release of **250 KJ/KJ per mol [14].**

**Catalysts:**

Catalysts play a vital role in technology, and their composition has evolved over time. In the past, catalysts were primarily composed of 1 to 5 wt.% palladium impregnated on silica, with alkali metal acetates used as activators. However, in modern catalysts, noble metals, particularly gold, are often utilized as enhancers. A typical example of a catalyst following the Bayer-type approach consists of 0.15 to 1.5 wt.% palladium and 0.2 to 1.5 wt.% gold, with a bulk content of 4 to 10 wt.%. The average lifespan of such catalysts ranges from 1 to 2 years.

## 7.1.4. Kinetics of Reaction:

In more recent studies the formation of vinyl acetate can be described conveniently by a power law kinetics involving only ethylene and oxygen:

**For the Primary Reaction:**

$$r_{\text{VA}} = k_1 \, p_{C2H4}^{\alpha1} \, p_{o2}^{\beta1}$$

where the partial pressures of ethylene and oxygen are directly proportional to the rate of vinyl acetate production (rVA). The reaction constant is $K2 = A_2e^{-E2/RT.}$

$\alpha_1$ and $\beta_1$ are partial reaction orders derived empirically, while $A_2$ is a pre-exponential factor. $P_{C2H4}$ is the partial pressure of ethylene and $P_{O2}$ is the partial pressure of oxygen.

**For Secondary Reaction:**

$$r_{\text{CO2}} = k_2 \, p_{C2H4}^{\alpha1} p_{o2}^{\beta1}$$

where $r_{\text{CO2}}$ is the rate of formation of vinyl acetate is directly proportional to the partial pressure of ethylene and the partial pressure of oxygen. $K2 = A_2e^{-E2/RT}$ is the reaction constant. $P_{C2H4}$ is partial pressure of ethylene and $P_{O2}$ is the partial pressure of oxygen; $\alpha_2$ and $\beta_2$ are partial reaction orders derived experimentally, $A2$ is a pre-exponential factor.

**Table 17:** Reaction Parameters [15]

| **Reactions** | **A** | **B** | **E (J/mol)** | **A (mol kg cat$^{-1}$ s$^{-1}$)** |
|---|---|---|---|---|
| **1** | 0.36 | 0.20 | 15000 | 0.000265 |
| **2** | -0.31 | 0.82 | 21000 | 0.000750 |

## 7.1.5. Design Equations:

$$\frac{\boldsymbol{W}}{\boldsymbol{FA0}} = \int_{0}^{\boldsymbol{XAout}} \frac{\boldsymbol{dXA}}{\boldsymbol{-rA}}$$

**For 1st Reaction:**

R = 8.314 KJ/kmol. K

T = 423.15K

P = 7 bar, 70000 Pa

$$\mathbf{K_1 = A_1 e^{-(E1/RT)}}$$

$K_1 = 0.000265 \exp\left(-\frac{15000}{RT}\right)$

$K_1 = 0.000265 \exp\left(-\frac{15000}{(8.314)(423.15)}\right)$

$K_1 = 3.728 * 10^{-6} \frac{kmol}{kg.cat.s}$

Now,

$r_{VA} = k_1 \, p_{C2H4}^{\alpha 1} \, p_{o2}^{\beta 1}$

whereas, from the design equation

Generate data curve between $X_A$ and $1/-r_A$ up to $X_A = 0.2$. These values have been taken from the book. (Chemical-process-design-alexandre)

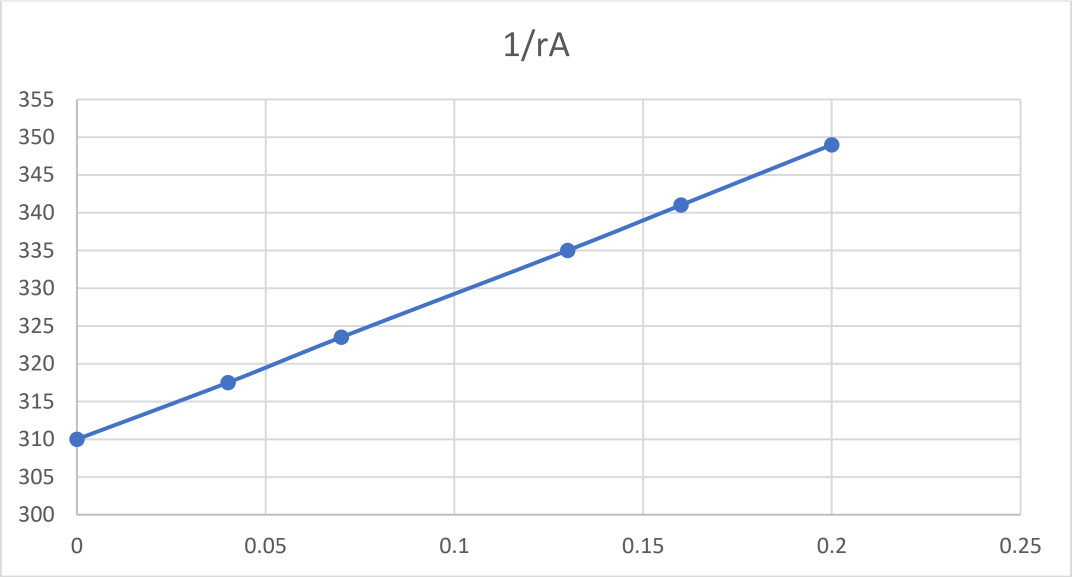


**Figure 6:** Rate of reaction for primary reaction

While $r_{vA} = 3.728*10^{-6}(0.4515*7)^{0.36}(0.02489*7)^{0.20}$

$$\mathbf{r_{VA} = 3.97*10^{-6}\frac{kmol\ bar}{kg.cat.s}}$$

Now by solving these values through Simpson 1/3rd rule for numerical integration we get:

$$\int_0^{0.2}\frac{dXA}{-rA} = \frac{0.05}{3}((f(0)+f(0.2)+4(f(0.05)+f(0.15)+2(f(0.1)+f(0.2))$$

$$\int_0^{0.2}\frac{dXA}{-rA} = 61.82\frac{kg.cat.s}{mol}$$

so,

$$\mathbf{F_{A0} = \frac{1000}{61.82}\frac{mol}{s}}$$

$\mathbf{F_{A0} = 162.52\ mol/s}$

Now from design equation,

$$\mathbf{W= \int_0^{0.2}\frac{dXA}{-rA} * F_{A0}}$$

W = 61.82 * 162.52

$\mathbf{W_2 = 10046.98\ Kg}$

For Volume of Catalyst,

$$\textbf{Volume of catalyst} = \frac{\textbf{Weight of catalyst}}{\textbf{Density of catalyst}}$$

Whereas, Density = 1000kg/$m^3$

Volume = 10046.98/1000

**Volume = $V_1$ = 10.046 $m^3$**

## For 2nd Reaction:

R = 8.314 KJ/kmol. K

T = 423.15K

P = 7 bar, 70000 Pa

$$\mathbf{K_2 = A_2 e^{-(E1/RT)}}$$

$K_2 = 0.00075 \exp\left(-\frac{21000}{RT}\right)$

$K_2 = 0.00075 \exp\left(-\frac{21000}{(8.314)(423.15)}\right)$

$K_2 = 1.917 * 10^{-6} \frac{kmol}{kg.cat.s}$

Now,

$r_{CO2} = k_2\, p_{C2H4}^{\alpha 1}\, p_{o2}^{\beta 1}$

whereas, from the design equation

Generate data curve between $X_A$ and $1/-r_A$ up to $X_A = 0.03$. These values have been taken from the book. (Chemical-process-design-alexandre)

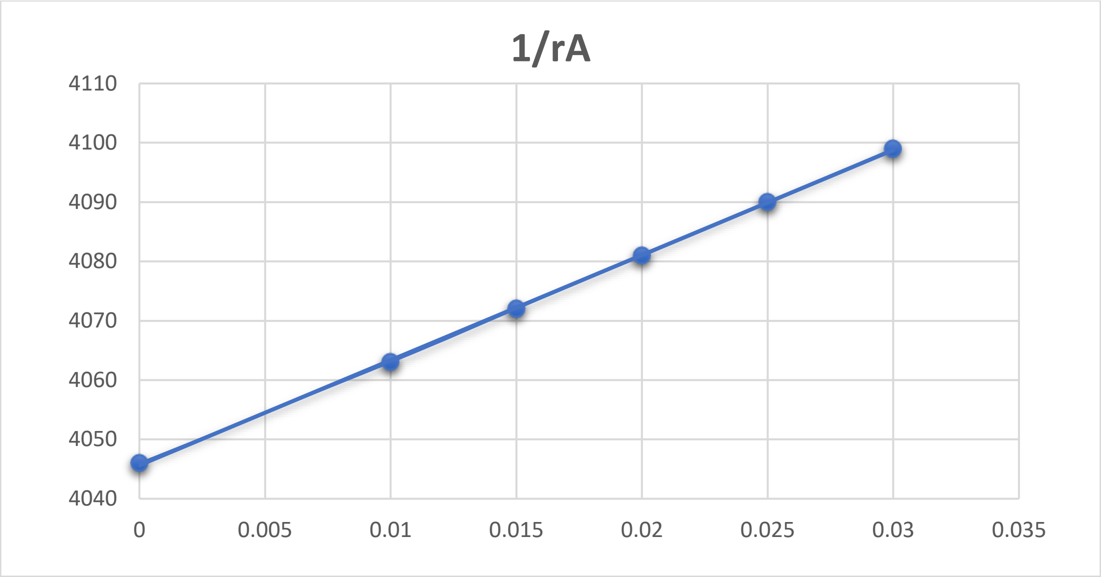


**Figure 7:** Rate of reaction of secondary reaction

While $r_{CO2} = 1.917*10^{-6} \frac{kmol}{kg.cat.s} (0.4515*7)^{-0.31}(0.02489*7)^{0.82}$

$$\mathbf{r_{CO2} = 3.20*10^{-7} \frac{kmol\ bar}{kg.cat.s}}$$

Now by solving these values through Simpson 1/3rd rule for numerical integration we get:

$$\int_0^{0.03} \frac{dXA}{-rA} = \frac{0.05}{3}((f(0) + f(0.03) + 4(f(0.005) + f(0.015) + f(0.025) + 2(f(0.01) + f(0.02) + f(0.03))$$

$$\int_0^{0.03} \frac{dXA}{-rA} = 110.776 \frac{cat.s}{mol}$$

So, from here we get,

$\mathbf{F_{A0} = 2.22\ mol/s}$

$$\mathbf{W = \int_0^{0.03} \frac{dXA}{-rA} * F_{A0}}$$

W = 110.776 * 2.22

$\mathbf{W_2 = 245.8\ Kg}$

For Volume of Catalyst,

$$\textbf{Volume of catalyst} = \frac{\textbf{Weight of catalyst}}{\textbf{Density of catalyst}}$$

Whereas, Density = 1000kg/m$^3$

Volume = 245.8/1000

**Volume = $V_2$ = 0.2458 $m^3$**

Total Volume = $V_1 + V_2$

**Total Volume of catalyst = V= 10.2918 $m^3$**

Void Volume = 0.55

Assuming,

L/D = 3

Whereas,

Volume = $\pi D^2/4$

Then by solving L/D with volume we get,

Diameter of Catalyst = 1.9811

Length of Catalyst = 5.9434

### 7.1.6. Shell and Tube Configuration:

All of this data of shell and tube configuration have been taken from the book (Chemical-process-design-alexandre) Chapter 10.

Outer Diameter = OD = 2 inch = 0.0508 m

Inner Diameter ID =1.76 inch = 0.0447m

Birmingham Wire Gauge = BWG = 11

Inner cross-sectional area of 1 tube:

Inner cross sectional flow area per tube= 2.433 $inch^2$ = 0.00157 $m^2$

Length of 1 tube = L = 13 ft = 4.0 m

Volume of 1 tube = cross sectional area per tube * Length of 1 tube

Volume of 1 tube = (0.00157 * 4.0)

Volume of 1 tube = 0.00628 $m^3$

No of tubes = $\frac{\text{Volume of reactor}}{\text{Volume of 1 tube}}$

No. of tubes = $\frac{\text{(volume of catalyst/ void volume)}}{0.00956}$

No. of tubes = $\frac{(10.2918/0.55)}{0.00628}$

**No. of tubes = 2500**

Triangular pitch = 1.25 * OD

Triangular pitch = 1.25*0.0508

**Triangular Pitch = $P_t$ = 0.0635m**

Diameter of bundle in mm = Db = do $(\frac{n}{k1})^{(1/n1)}$

Whereas,

Do = outer diameter

N= No. of tubes

So,

**For Triangular pitch;**

K1 = 0.319

N1 = 2.142

So,

Db = 2954.33 mm

From figure 12.10 of book (RK SINNOT)

Clearance = 127 mm

Inside diameter of shell = $D_b$ + Clearance

Inside diameter of shell = 2954.33 + 127 = 3081.22 mm/1000 = 3.081m

For 20 percent extra space

Inside diameter of shell =3.081m

Thickness t = 17.7mm

Shell outside Diameter = 3.1105m

Length of shell= 3D = 3*3.1105 = 9.3315m

Now, calculating

Original diameter of reactor = 3.3015 m

Original length of reactor = 3D = 9.9044 m

**Diameter and Area of Shell:**

The diameter of the shell (total bundle of tubes diameter) can be calculated by the formula:

$$\mathrm{D_b} = \mathrm{D_o}\frac{(Number\ of\ Tubes)^{\frac{1}{n}}}{K_1}$$

Where,

$K_1$ and n are constant values obtained from the choice of pitch:

Triangular pitch is selected as it gives a compact arrangement, resulting in smaller shell.

Pt = 1.25$D_0$

Pt = 1.25 × 0.0025 = 0.003125 m

For 1 shell pass, 1 tube pass: K1 = 0.319 and n = 2.142

$$\mathrm{D_b} = 0.0025\ \frac{(\ 1920)^{\frac{1}{2.142}}}{0.319}$$

$$\mathrm{D_b} = 0.2673\mathrm{m}$$

Clearance = 25% of $D_0$ = 0.000625 m

Shell diameter:

Shell diameter $= \mathrm{D_b}$+ Clearance

$$\text{Shell diameter} = 0.2673 + 0.000625$$

$$\text{Shell diameter} = 0.2679\ \mathrm{m}$$

**Area of Shell:**

$$\text{Area of Shell} = \frac{\pi(D\ of\ Shell)^2}{4}$$

$$\text{Area of Shell} = \frac{\pi(3.1105)^2}{4}$$

$$\text{Area of Shell} = 7.59\text{m}^2$$

Outer area of tubes:

$$\text{Area of tubes} = \frac{\pi \text{ x } Nt \text{ x } (Dt)^2}{4}$$

$$\text{Area of tubes} = \frac{\pi \text{ x } 1920 \text{ x } (0.0025)^2}{4}$$

$$\text{Area of tubes} = 0.00942 \text{ m}^2$$

Area of shell is greater than area of tubes, so the design is satisfactory.

$$\text{Aspect ratio} - \text{L/D ratio} = \frac{9.3315}{3.1105}$$

L/D ratio = 3

The L/D ratio is not extremely high hence capital cost is reduced as well. For tubular reactors, the aspect ratio is around 8.

**Residence Time:**

$$\text{Residence Time} = \frac{volume\ of\ reactor}{volumetric\ flow\ rate}$$

$$\tau = \frac{V}{v_o}$$

$$\tau = \frac{10.2918}{2109.133}$$

Residence Time = 0.00487 hr. = 17.56 sec

### 7.1.7. Mechanical Design of Reactor:

For cylindrical shell, minimum wall thickness;

T(m) = $\frac{Pri}{SEj - 0.6P} + Cc$

Whereas,

Pressure = 7 bar

Joint Efficiency = Ej = 1

Maximum Allowable stress = S = 94500 KPa

Corrosion Allowance = Cc = 0 (Assume)

Radius of Shell = ri = 3.1105/2 = 1.555m

Now calculating,

T = $\frac{7*1.555}{94500*1-o.6*7}+0$ = 0.0011519m = 11.51 mm

### 7.1.8. Pressure Drop in Tube Side:

$$\frac{\Delta p}{L}=\frac{150\mu(1-\varepsilon)^2\mu0}{\varepsilon^3(Particle\ diameter)^2}+\frac{1.75(1-\varepsilon)\ \rho\mu0}{\varepsilon^3(Particle\ diameter)^2}$$

Whereas,

$\varepsilon$ = Void Fraction = 0.45

L = Length of bed = 5.9434m

$\rho$ = Density (Assume) = 10kg/m$^3$

$\mu$= Viscosity = 8.3637 pa.s

$\mu$0= Super facial velocity = 0.1945 m/sec

Particle diameter = 5 mm

So, by calculation we get,

$$\Delta p=\frac{150*8.3637*(1-0.45)^2*0.1945}{(0.45)^3*(5)^2}+\frac{1.75*(1-0.45)*\ 10*0.1945}{(0.45)^3*(5)^2}*5.9434$$

**$\Delta p$ = 1929614 Pa = 1929.614 KPa = 1.9 Bar**

## 7.1.9. Specification Sheet:

**Table 18:** Specification sheet of reactor

| **Identification** | |
|---|---|
| **Item** | Reactor |
| **No. Required** | 1 |
| **Type** | Packed Bed Multi Tubular Reactor |
| **Operating Temperature** | 423.15 |
| **Pressure** | 7 Bar |
| **Time of Contact** | 17.23 sec |
| **Reactor Volume** | 85.05 $m^3$ |
| **Reactor Diameter** | 3.301 |
| **Reactor Length** | 9.904 |
| **Outside diameter of tube** | 0.0508 m |
| **Length of 1 tube** | 4.0 m |
| **Volume of 1 tube** | 0.00628 $m^3$ |
| **Total Tubes** | 2500 |
| **Pressure Drop** | 1929 KPa |

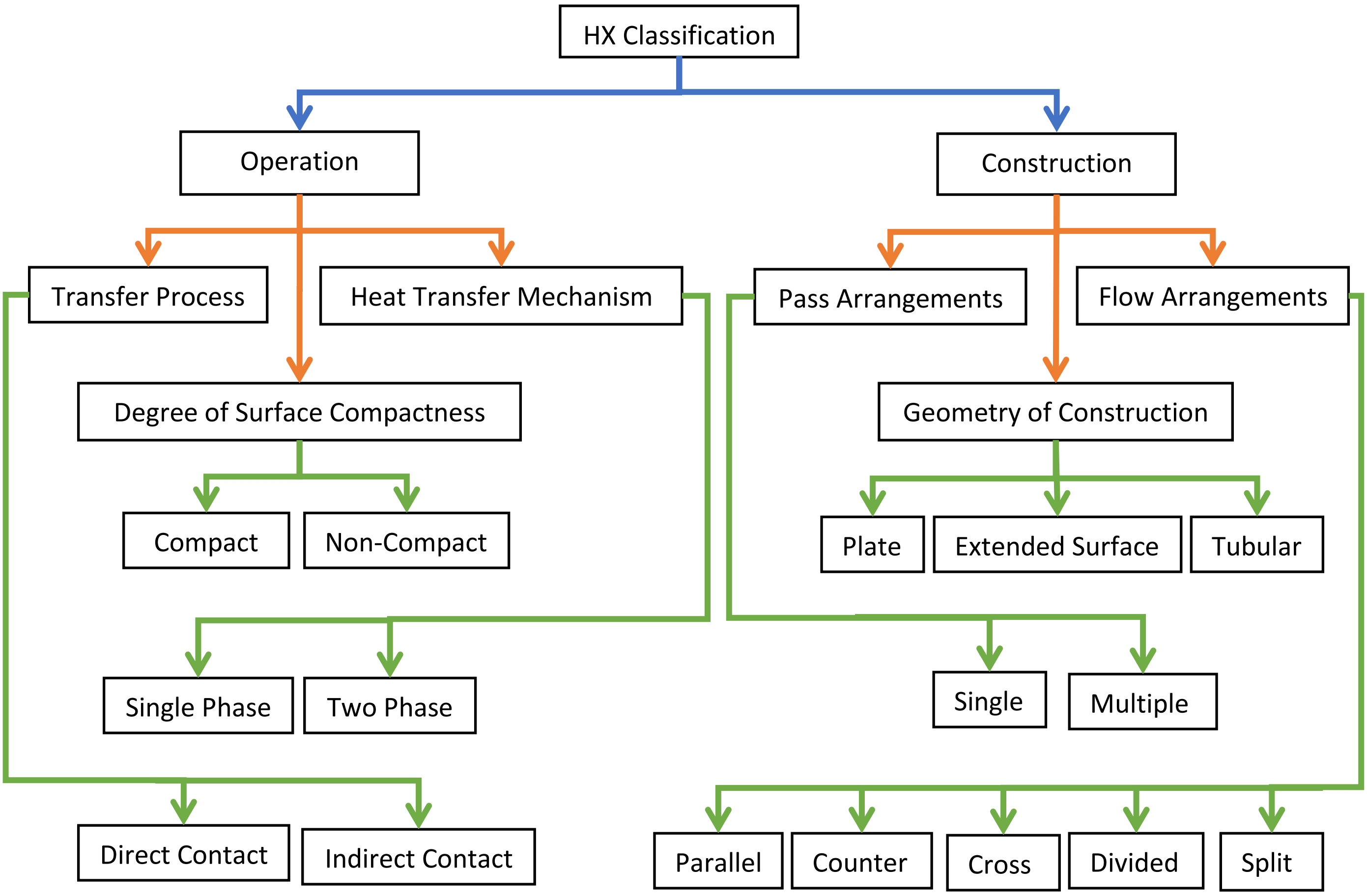
## 7.1. Heat Exchanger:

- A heat exchanger (HX) is a device that transfers thermal energy between two fluids. It is a common component in many industrial and commercial applications, including boilers, coolers, cooling water heat exchangers, evaporators, and condensers.

- Two fluids with varying temperatures that are separated from one another by a conducting medium make up the basic building blocks of a heat exchanger. The most common design uses two fluids, one of which circulates inside the tubes and the other surrounds them. The heat is transferred from the heated fluid to the cool fluid through a combination of conduction and convection.

- The surface area of the heat transfer surface, the temperature differential between the fluids, and the kind of conducting media are only a few variables that affect how efficient a heat exchanger is. Heat exchangers are a crucial part of numerous industrial processes and are crucial for energy efficiency and conservation.

### 7.2.1. Classification Of Heat Exchangers:



## 7.2.2. Selection of Heat Exchanger:

**Table 19:** Selection of Heat Exchanger

| Type | Significant feature | Applications that work best | Limitations | Comparative cost in carbon steel construction, approximation |
|---|---|---|---|---|
| **Fixed tube sheet** | The tube sheets are rigidly attached to the shell. | Condensers, liquid-liquid, gas-gas, gas-liquid, cooling and heating, horizontal or vertical reboiling | Temperature difference at extremes of about 200 °F. Due to differential expansion. | 1.0 |
| **Floating head or tube sheet (removable and non-removable bundles)** | Floating tube sheets allow tubes to expand and contract freely preventing stress and making the bundle removeable. | Extreme Temp. differences above 200 °F filthy fluids required cleaning on both inside or outside whether horizontally or vertically. | Internal gaskets present at leakage risk fluid ability to control floating portion on the shell. | 1.28 |
| **U-tube;**<br>**U-Bundle** | There is only one tube sheet required in the form of U shaped curved. Bundle can be eliminated | High temp. differences which may necessitates adding expansion capacities to fixed tube system | Bends must be done carefully to prevent mechanical damage and the risk of rupture. Inside of bends may erode due to tube side velocities. | 0.9-1.1 |
| **Double pipe** | In a shell and tube heat exchanger, each tube is | In banks for larger applications, or in relatively | Finned tubes are suitable for high heat transfer | 0.8-1.4 |

| | | | | |
|---|---|---|---|---|
| | surrounded by its own shell. The shell-side fluid flows through the annular space, transferring heat to the finned tube | small transfer areas. particularly well suited for high tube pressures (higher than 400 psig). | applications. However, they are costly and space-consuming. | |
| **Pipe coil** | A pipe coil submerged in water is the simplest type of heat exchanger. It is simple, inexpensive, and versatile, but not very efficient or suitable for high-heat applications. | Low heat burdens on sensible transfer, or condensation. | A low transfer coefficient requires a large heat exchanger for a high heat load. | 0.5-0.7 |
| **Plate and frame** | Thin metal plate heat exchangers are compact and easy to clean. | Fluids with high heat transfer, slurries, and viscosity. | The maximum temperature for plate heat exchangers is between 350 and 500°F, which makes them unsuitable for boiling or condensing. They cannot be utilized for gas-gas applications; only liquid-liquid applications | 0.8-1.5 |

**Shell and Tube Heat Exchanger:**

The effective, dependable, and adaptable method of transferring heat between two fluids is the shell and tube heat exchanger. They are the most prevalent type of heat exchanger used in industry and have a wide range of uses, including food processing, chemical processing, and the production of electricity.

A shell, a bundle of tubes, and a tube sheet make up a shell and tube heat exchanger. The tubes are kept in the shell, which is a sizable cylindrical container. The hot fluid is poured into the tubes, and the cool fluid is poured into the shell. Through the tube walls, heat is transmitted from the hot fluid to the cool fluid.

Because they may be used to transfer heat between a wide range of fluids and function at a wide range of temperatures and pressures, shell and tube heat exchangers are widely employed. Additionally, they are comparatively simple to maintain and fix.

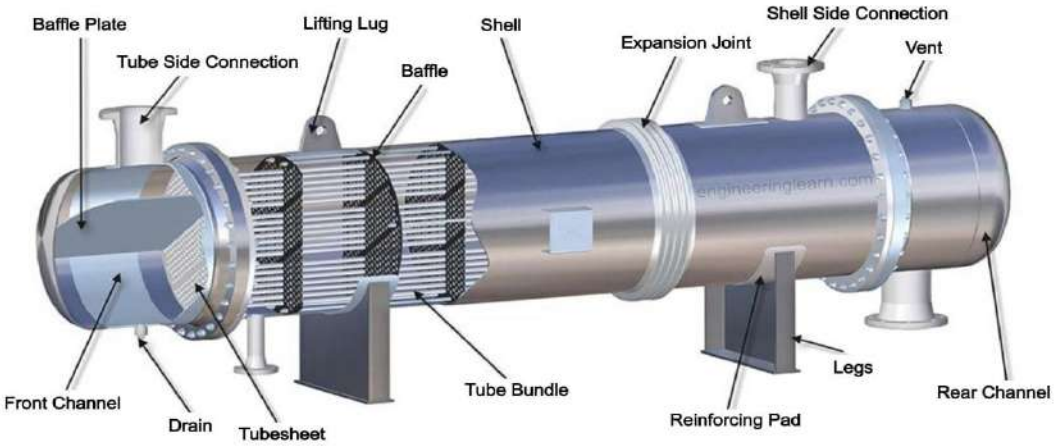


**Figure 8:** Shell and Tube HX

### 7.2.3. Types of the shell and tube heat exchangers:

Heat exchangers have been developed with different approaches to these four fundamental design factors. Three principal types of heat exchangers

- U-tube exchangers
- Fixed tube-sheet exchangers
- Floating head exchangers

## U -Tube Exchangers:

U-shaped tubes are used in U-tube heat exchangers, a form of heat exchanger, to transfer heat between two fluids. They are utilized in many different applications, including as power production, chemical processing, and food processing. They are small and effective.

U-shaped tubes are used in U-tube heat exchangers to transfer heat between two fluids. They are effective and little. They are employed in a number of processes, such as food processing, chemical processing, and power generation.

## Straight or Fixed tube Exchangers:

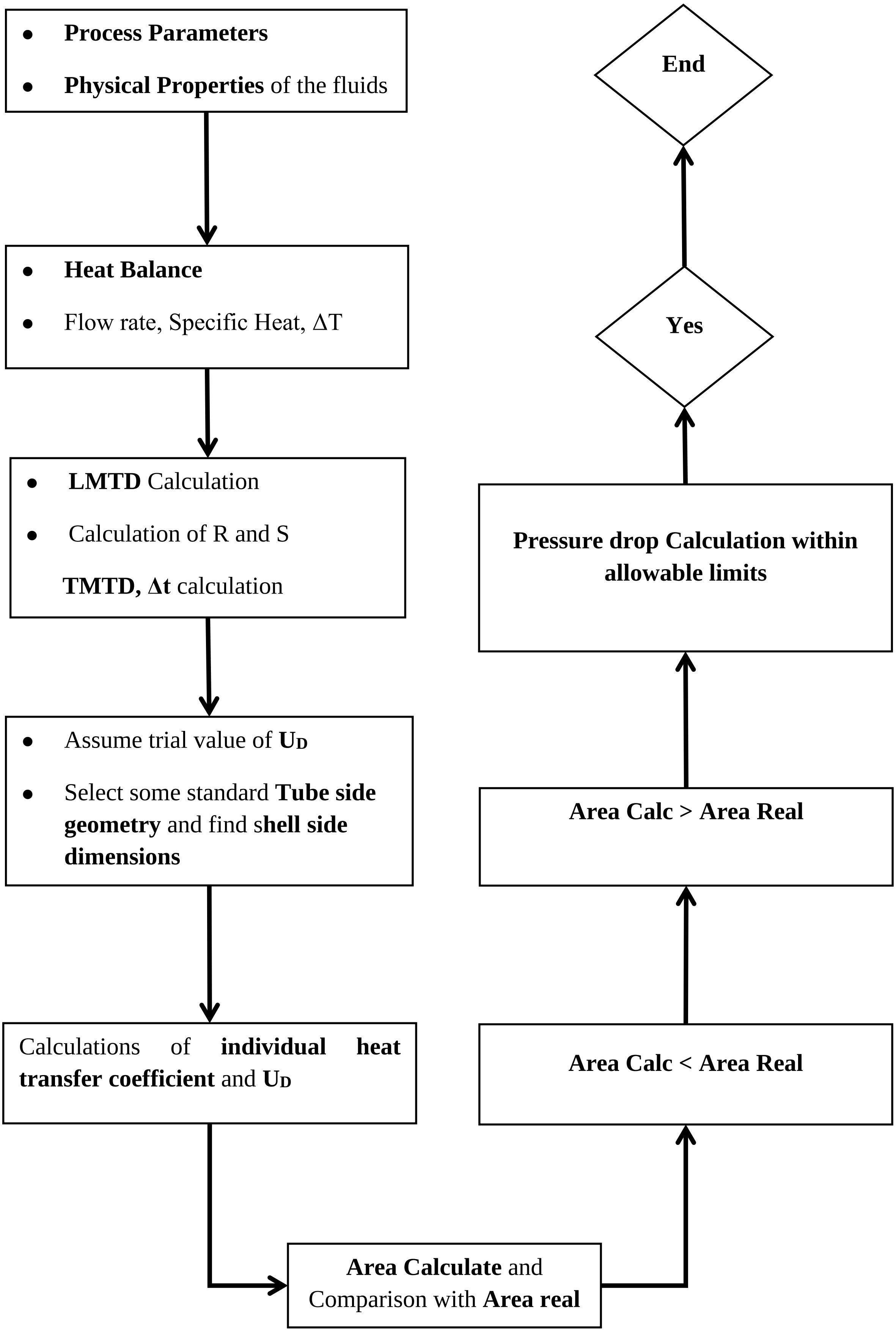
Straight tubes are used in straight-tube heat exchangers to transfer heat from one fluid to another. They are made to deal with applications involving heavy fouling fluids or temperature cross situations. It is advantageous to handle high fouling fluids with them because the head assemblies can be taken apart and the tubes may be mechanically cleaned.

## Floating-head type Exchanger:

A form of shell-and-tube heat exchanger that can withstand high temperatures and pressures are floating head heat exchangers. By enabling the tube bundle to move within the shell as it expands and contracts, they are intended to prevent thermal stress and fatigue.

To satisfy the needs of our process, we have chosen a fixed tube sheet 1-2 shell and tube heat exchanger.

### 7.2.4. Heat Exchanger Design Algorithm



### 7.2.5. Selection of basic type of Heat Exchanger:

The following qualitative traits are used to select fixed tube shell and tube heat exchangers:

- TEMA and ASME offer well-established codes and standards.
- Comes in the broadest range of materials
- Several years of good service
- Thermodynamic and hydraulic properties
- Material compatibility
- Operational upkeep and cleaning
- Rules and considerations relating to SHE
- High volume and weight to heat transfer area ratios.
- The product comes in the most styles and sizes.
- Mechanical adversity

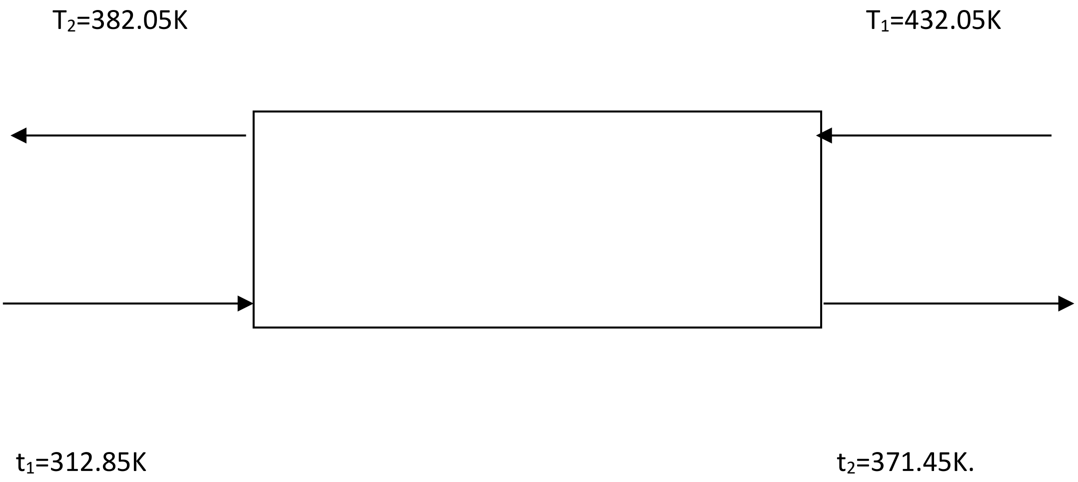


**Figure 9:** Shell and Tube HX

### 7.2.6. Cp Calculation:

**For Gas Stream:**

The correlation for heat capacity of gas is a series expansion in temperature.

$$Cp = a + bT + cT^2 + dT^3 + eT^4$$

(Chemical Properties Handbook, Carl L. Yaws)

Here a, b, c, d, e is regression coefficients for chemical compound

**Table 20:** Heat capacity coefficients for Gases

| **Components** | **Heat capacity coefficients for Gases** | | | | |
|---|---|---|---|---|---|
| | **a** | **b** | **c** | **d** | **e** |
| **Acetic acid** | 34.85 | 0.037626 | 0.00028311 | -3.067E-07 | 9.2646E-11 |
| **Water** | 33.933 | -0.0084186 | 0.000029906 | -1.7825E-08 | 3.6934E-12 |
| **Oxygen** | 29.526 | -0.0088999 | 0.000038083 | -3.2629E-08 | 8.8607E-12 |
| **VAM** | 27.664 | 0.23366 | 0.000062106 | -1.6972E-07 | 5.7917E-11 |
| **Ethylene** | 32.083 | -0.014831 | 0.00024774 | -2.3766E-07 | 6.8724E-11 |
| **Carbon Dioxide** | 27.437 | 0.042315 | -0.000019555 | 3.9968E-09 | -2.9872E-13 |

| | | | |
|---|---|---|---|
| **TOTAL Cold side Cp at average temperature 342.15 K =** | 1646.0357 J/Kg. K | **TOTAL hot side Cp at average temperature 407.05 K =** | 1177.600774 J/Kg. K |

### 7.2.7. Viscosity Calculation:

**For Gas Stream:**

The correlation for viscosity of gas is a series expansion in temperature.

$$\textbf{Viscosity} = a + bT + cT^2$$

(Chemical Properties Handbook, Carl L. Yaws)

Here a, b, c, is regression coefficients for chemical compound

**Table 21:** Data of viscosity

| Components | a | b | c | Viscosity COLD | Viscosity HOT |
|---|---|---|---|---|---|
| **Carbon Dioxide** | 11.811 | 0.49838 | -0.00010851 | 167.2290386 | 200.3791782 |
| **Ethylene** | -3.985 | 0.38726 | -0.00011227 | 113.6154053 | 137.7008552 |
| **Acetic Acid** | -28.66 | 0.2351 | 0.00022087 | 75.46075706 | 107.3854225 |
| **VAM** | -7.462 | 0.30466 | 0.000057544 | 101.5719266 | 129.2525214 |
| **Water** | -36.826 | 0.429 | -0.0000162 | 105.6981376 | 138.8552688 |
| **Oxygen** | 44.224 | 0.562 | -0.000113 | 220.5417558 | 258.4840709 |

| | | | |
|---|---|---|---|
| **TOTAL Cold side Viscosity at average temperature 342.15 K =** | 1.13615E-05 kg/ms | **TOTAL hot side Viscosity at average temperature 407.05 K =** | 9.72057E-05 kg/ms |

## 7.2.8. Thermal Conductivity Calculation:

**For Gas Stream:**

The correlation for thermal conductivity of gas is a series expansion in temperature.

$$\text{Thermal Conductivity} = a + bT + cT^{2}$$

(Chemical Properties Handbook, Carl L. Yaws)

Here a, b, c, is regression coefficients for chemical compound

**Table 22:** Data of Thermal Conductivity

| Components | a | b | c | Thermal Conductivity COLD | Thermal Conductivity HOT |
|---|---|---|---|---|---|
| **Carbon Dioxide** | -0.012 | 0.00010208 | -2.2403E-08 | | 0.026592478 |
| **Ethylene** | -0.00123 | 0.000036219 | 1.2459E-07 | 0.0250653 | 0.035405145 |
| **Acetic Acid** | 0.00234 | -6.5956E-06 | 1.2439E-07 | | 0.021127511 |
| **VAM** | -0.00846 | 0.000058704 | 1.7678E-08 | | 0.019023819 |
| **Water** | 0.00053 | 0.000047093 | 4.9551E-08 | | 0.028700202 |
| **Oxygen** | 0.00121 | 0.000086157 | -1.3346E-08 | | 0.034745459 |

**TOTAL Cold side Thermal conductivity at average temperature 342.15 K =** 0.0250653 W/mK

**TOTAL hot side Thermal conductivity at average temperature 407.05 K =** 0.165594615 W/mK

## 7.2.9. Thermal Rating:

The design calculations or thermal rating of a shell and tube exchanger comprises of the following steps.

Inlet temperature of the Cold stream = $t_1$ = 312.85K

Outlet temperature of the Cold stream = $t_2$ = 371.45K.

Inlet temperature of hot stream = $T_1$ = 432.05K

Outlet temperature of hot stream = $T_2$ = 382.05K

Mass flow rate of hot stream = $m_h$ = 6.2489 Kg/s

| | |
|---|---|
| Specific heat capacity of the hot stream | = $Cp_{avg}$ =1177.600 J/Kg. K |
| Specific heat capacity of the cold stream | = $Cp_{avg}$ = 1629.58 J/Kg. K |
| Mass flow rate of the cold stream | = $m_c$ =? |
| Viscosity of the Cold stream | = $\mu_{avg}$ = 0.0000113615 Kg/ms |
| Viscosity of the Hot stream | = $\mu_{avg}$ = 0.0000972 Kg/ms |
| Thermal Conductivity of the Cold stream | = $k_{avg}$ = 0.0250653 w/m. K |
| Thermal Conductivity of the Hot stream | = $k_{avg}$ = 0.165594 w/m. K |

## Heat load Calculations:

$$\boldsymbol{Q = mC_p\Delta T}$$

$$Q = 6.2489 \ * 1177.600 * (432.05 - 382.05)$$

$$\boldsymbol{Q = 366961.0285\ Watt}$$

## Mass flow rate of utility stream:

$$\mathbf{Q = mC_p\Delta T}$$

$$m = \frac{366961.0285}{1629.58 * (371.45 - 312.85)}$$

$$\mathbf{m = 3.844074\ Kg/s}$$

## LMTD:

$$\mathbf{\Delta T_m = \frac{(T_1 - t_2) - (T_2 - t_1)}{ln\frac{(T_1 - t_2)}{(T_2 - t_1)}}}$$

$$\Delta T_m = \frac{(432.05 - 371.45) - (382.45 - 312.85)}{ln\frac{(432.05 - 371.45)}{(382.45 - 312.85)}}$$

$$\mathbf{\Delta T_m = 64.9049\ K}$$

## TMTD:

$R = \frac{T_1 - T_2}{t_2 - t_1} = 0.853242$ $\qquad$ $S = \frac{t_2 - t_1}{T_1 - t_1} = 0.491611$

$Ft = 0.85$ so, it is 1 shell pass and 2 or more tube pass

$$TMTD = LMTD * Ft$$

$$TMTD = 55.0841\ K$$

## Assumed calculations:

Value of $U_D$ assumed

**$U_D$ = 425.8698 W/m$^2$.K**

Now, Assume ¾ inch OD of tube, 16ft length and 16 BWG

## Heat transfer area:

$$\mathbf{A = \frac{Q}{U_D \Delta t}}$$

$$A = \frac{366961.0285}{425.8698 * 64.9049}$$

**A = 15.64286 m$^2$**

Tube length = 16ft = 4.876562 m

Tube OD = 0.75inch = 0.019045 m

Tube ID = 0.62inch = 0.015744 m

Shell ID = 10 inch = 0.253936 m

Flow area per tube Sq inch at 16 BWG = af = 0.302in$^2$ = 0.000195 m$^2$

External area of tube = a = 0.1963ft = 0.05983m

Number of tube pass = n = 2

Pitch = 1inch = 0.0253936m

## Number of Tubes

$$\mathbf{N = \frac{A}{aL}}$$

$$a = 0.1963\ ft = 0.05983\ m \quad \left(from\ table\ at\ \frac{3}{4} inch\ OD\ of\ tube\right)$$

$$N = \frac{15.64286}{0.05983 * 4.8765}$$

$$\boldsymbol{N = 53.61525}$$

Now the actual number of tubes are; (from table in book)

$$\mathbf{N_{actual} = 52\ tubes}$$

**Area** **real:**

$$Areal = N * a * L$$

$$Areal = 52 * 0.05983 * 4.8765$$

$$\mathbf{Areal = 15.17159m^2}$$

### 7.2.10. Tube Side Calculations:

Since my cold stream flow rate is lower than hot stream so cold stream will be in tube side and all cold stream related values will be used

## Flow area:

$$a_t = \frac{N * a_f}{n}$$

$$\mathbf{a_t = 0.005063244m^2}$$

## Mass velocity:

$$G_t = \frac{m}{a_t}$$

$$G_t = \frac{3.8142}{0.005063244}$$

$$\boldsymbol{G_t = 753.3164\, {}^{kg}/_{sec.m^2}}$$

## Reynolds No.:

$$Re = \frac{D * G_t}{\mu}$$

$$\mathbf{Re = \ 1043897}$$

## Prandtl Number:

$$Pr = \frac{Cp * \mu}{k}$$

$$\mathbf{Pr = \ 0.73840}$$

## Nusselt Number:

$$Nu = 0.023Re^{0.8}Pr^{0.33}\frac{\mu}{\mu w}^{0.14}$$

Since, $\frac{\mu}{\mu w}^{0.14} = 1$

So,

$$\mathbf{Nu = 1358.91}$$

## Heat Transfer coefficient:

$$hi = \frac{Nu * k}{ID\ of\ tube}$$

**$h_i$ = 2163.455 W/m$^2$.K**

### 7.2.11. Shell Side Calculations:

## Tube Clearance:

$$\mathrm{C = P_T - OD\ of\ tube}$$

$$\mathrm{C = 0.0253936 - 0.019045}$$

$$\mathbf{C = 0.006348\ m}$$

## Baffle Spacing:

$$B = IDof\ shell - (ID\ of\ shell * \frac{1}{5})$$

$$B = 0.253936 - (0.253936 * \frac{1}{5})$$

$$\mathbf{B = 0.2031488\ m}$$

## Flow area:

$$a_s = \frac{Ds * C'B}{P_T}$$

$$a_s = \frac{0.253936 * 0.006348 * 0.2031488}{0.0253936}$$

$$\boldsymbol{a_s = 0.012897 m^2}$$

## Mass velocity

$$G_s = \frac{m}{a_s}$$

$$G_s = \frac{6.2489}{0.012897}$$

$$\boldsymbol{G_s = 484.5348\ {}^{kg}/_{sec\,m^2}}$$

## Equivalent Diameter:

$$D_E = 8(0.43\ P_T^2 - 1/8\ \Pi\ d_o^2) / \Pi\ d_o$$

$$De = \frac{4[0.5(P_T)0.86(P_T) - (\frac{лdo^2}{8})}{\left(\frac{лdo}{2}\right)}$$

$$\mathbf{De = 0.018048\ m}$$

## Reynolds No.:

$$Re = \frac{D_e G_s}{\mu}$$

$$\mathbf{Re = 89966.89}$$

## Prandtl Number:

$$Pr = \frac{Cp * \mu}{k}$$

$$\mathbf{Pr = 0.689395}$$

## Nusselt Number:

$$Nu = 0.36Re^{0.55}Pr^{0.33}\frac{\mu}{\mu w}^{0.14}$$

$\frac{\mu}{\mu w}^{0.14} = 1$ So,

$$\boldsymbol{Nu} = \mathbf{168.9439}$$

## Shell side coefficient:

$$ho = \frac{Nu * k}{De}$$

$$\boldsymbol{ho} = \mathbf{1550.112 W/m^2.K}$$

## For coefficient correction:

$$hio = hi\frac{ID\ of\ tube}{OD\ of\ tube}$$

$$\boldsymbol{hio} = \mathbf{1788.456}\,\mathbf{W/m^2.K}$$

## Clean overall coefficient:

$$U_C = \frac{h_{io}h_o}{h_{io} + h_o}$$

$$\boldsymbol{U_C} = \mathbf{830.388}\ \mathbf{W/m^2.K}$$

## Design overall coefficient:

$$\frac{1}{U_D} = \frac{1}{U_C} + Rdi + Rdo$$

Rdi = 0.00053 $m^2$ K/W (value for light organic hydrocarbon gas)

Rdo = 0.00061 $m^2$ K/W (value for Solvent vapors)

$$\boldsymbol{U_D} = \mathbf{426.5745}\ \mathbf{W/m^2.K}$$

This value is sufficiently close to the assumed the value of 425.8698 W/$m^2$.K to be acceptable.

## Calculated Area:

$$\mathbf{A_{cal}} = \frac{\mathbf{Q}}{\mathbf{U_D} * \mathbf{TMTD}}$$

$$\mathbf{A_{cal}} = \mathbf{15.61702m^2}$$

Hence, $A_{cal}$ is almost equal to $A_{real}$

### 7.2.12. Pressure Drop Calculations:

## Condition:

f = Friction factor can be calculated using following equation.

For laminar region (NRe < 2100)

f = 16/NRe

For turbulent region (NRe > 2100)

If NRe < 20000, f = 0.316 NRe $^{(-1/4)}$

If NRe > 20000, f = 0.184 NRe $^{(-1/5)}$

## Tube side:

For Reynolds number = 1043897

Friction factor for tube side, f = 0.184 NRe $^{(-1/5)}$ = 0.01151

Tube diameter, $D_t$ = 0.1934 ft

Number of passes, n = 2

Mass Velocity, $G_t$ = 418492 lb./hr. sqft

Tube length, L = 16 ft

S = 0.491611

$$\Delta P_t = \frac{f {G_t}^2 L n}{5.22 * 10^{10} * D_e * s}$$

$$\Delta P_t = 12.42139\, psi$$

## Shell side

Reynolds No, Re = 89966.89

Mass velocity, $G_s$ = 301856.832 lb/hr. sqft

Friction factor, f = 0.184 NRe $^{(-1/5)}$ = 0.018793

S = 0.491611

No. of crosses, N+1 = [(Ls/2*Bs)-1] +1 = 12

Shell Diameter, $d_s$ = 10 inch

Equivalent Diameter, $D_e$ = 0.891 ft

$$\Delta P_s = \frac{f {G_s}^2 d_s (N+1)}{5.22 * 10^{10} * D_e * s}$$

$$\Delta P_s = 8{,}986844\ psi$$

### 7.2.13. Specification Sheet:

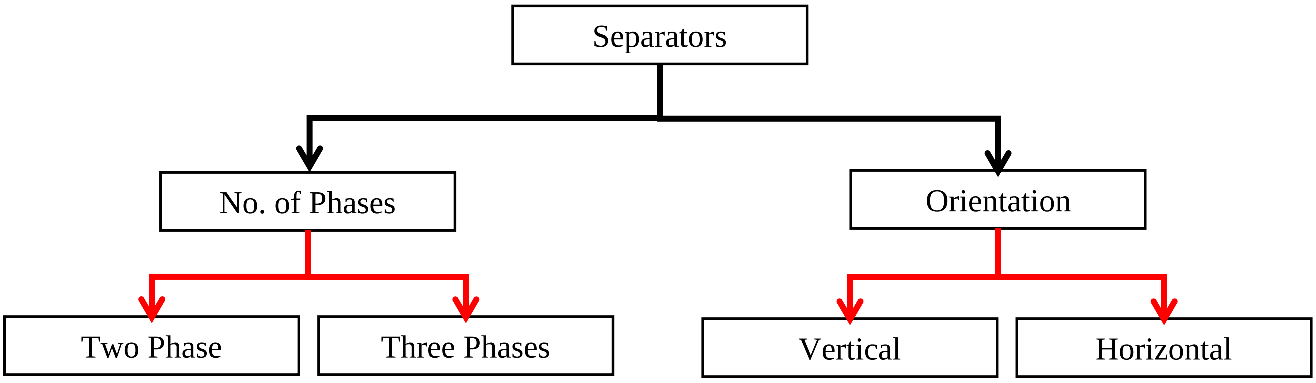
**Figure 10:** Specification of HX

| | |
|---|---|
| **Shell Diameter (Ds)** | 10 inches |
| **Number of Total Tubes** | 52 |
| **Pressure Drop (Shell side)** | 8.98psi |
| **Pressure Drop (Tube side)** | 12.42psi |
| **Area of Heat Exchanger** | 15.610m$^2$ |
| **Overall Heat Transfer Coefficient ($U_D$)** | 425.8698 W/m2.K |

## 7.2. Flash Separator:

A flash column or two-phase separator is a device that uses forces to separate two phases of a fluid. The forces can be centrifugal, primary, or electromotive. Flash columns and two-phase separators are used in a variety of applications, including oil and gas production, chemical processing, water treatment, and wastewater treatment

### 7.2.1. Classification of Separators:



**Other Types:**

- Spherical Separators
- Centrifugal Separators
- Venturi Separators
- Double-Barrel Horizontal Separators
- Horizontal Separator with a Water Pot
- Filter Separator
- Scrubbers
- Slug Catchers

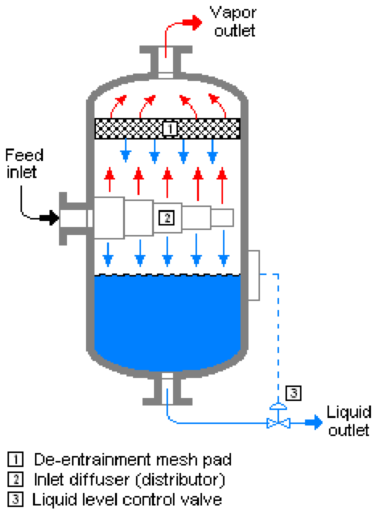
**Table 23:** Types of Separators

| Type | Description |
|---|---|
| **Vertical Gas-Liquid Separator** | Vertical gas-liquid separators separate gas and liquid mixtures. They are available in various sizes and configurations. They are a reliable and cost-effective way to separate gas and liquid mixtures |
| **Horizontal Gas-liquid Separator** | Vertical gas-liquid separators are used for gas-rich mixtures, while horizontal gas-liquid separators are used for liquid-rich mixtures. Vertical separators are larger and more expensive, while horizontal separators are smaller and less expensive. |

## Selection Criteria:

1. The selection of either a Horizontal or Vertical flash column is typically based on the density of the liquid or vapor. However, the actual determining factor for choosing between Horizontal or Vertical flash columns is the L/D ratio.
2. The design steps for both vertical gas-liquid separators and horizontal gas-liquid separators are nearly identical.
3. A vertical two-phase separator is utilized when the L/D ratio falls within the range of 3-5.
4. If the L/D ratio does not fall within this range, the next option is to consider a Horizontal two-phase separator.
5. A Horizontal two-phase separator is chosen when the L/D ratio exceeds 5

## 7.2.2. Diagram:



## 7.2.3. Design Steps:

1. Determination of density of vapors and liquids
2. Determination for maximum velocity
3. Determination of VFR of liquids and vapors
4. Determination of Area
5. Determination of Diameter
6. Determination of Volume of liquid
7. Determination of total height
8. Determination of L/D ratio

## 7.2.4. Calculations of Density of liquid and vapors:

**For liquid:**

Average density of liquid phase = mass fraction of component * density of component

$$\rho_{liquid} = x_{components} * \rho_{component}$$

$\rho_{liquid} = (x_{vam} * \rho_{vam}) + (x_{co2} * \rho_{co2}) + (x_{o2} * \rho_{o2}) + (x_{H2O} * \rho_{H2O}) + (x_{CH3COOH} * \rho_{CH3COOH}) + (x_{C2H4} * \rho_{C2H4})$

$\rho_{liquid} = (0.2689 * 934) + (0.0221 * 1101) + (0.0002659 * 1141) + (0.0699 * 997) + (0.6102 * 1049) + (0.02839 * 1.18)$

$\boldsymbol{\rho_{liquid} = 985.6116921\ kg/m^3}$

**For vapors:**

$PV = nRT$

$P\frac{m}{\rho} = nRT$

$\frac{P\ n\ M}{\rho} = nRT$

$\frac{P\ n\ M}{n\ R\ T} = \rho_{vap}$

$\rho_{vap} = \frac{P\ M}{R\ T}$

So, firstly we need to calculate the Molar Mass of Vapor Phase;

Molar Mass of Vapors = mass fraction of component * molar mass of component

$M_m = (x_{vam} * M_{vam}) + (x_{co2} * M_{co2}) + (x_{o2} * M_{o2}) + (x_{H2O} * M_{H2O}) + (x_{CH3COOH} * M_{CH3COOH}) + (x_{C2H4} * M_{C2H4})$

$M_m = (0.016400521 * 86.09\ g/mol) + (0.440867513 * 44.01\ g/mol) + (0.03196898 * 16 g/mol) + (0.000957367 * 18\ g/mol) + (0.005277229 * 60.052\ g/mol) + (0.50452839 * 28.05\ g/mol)$

$M_m = 1.411920874 + 19.40257923 + 0.511503685 + 0.017232611 + 0.316908137 + 14.15202133$

**$M_m$ = 35.81216587 g/mol**

$$\rho_{vap} = \frac{\mathrm{P\,M}}{\mathrm{R\,T}}$$

$$\rho_{vap} = \frac{4.18\ (\mathrm{bar}) * 35.81(\mathrm{g/mol})}{8.314472\mathrm{e}^{-5}\ (\mathrm{m}^3\ \mathrm{bar}\ /\mathrm{K\ mol}) * 308.5\ (\mathrm{K})}$$

$$\rho_{vap} = \frac{172.2461\ \mathrm{g}}{0.02565\ m3}$$

**$\rho_{vap}$ = 6715.2475 g/mol**

$$\rho_{vap} = \frac{172.2461\ \mathrm{g/m3}}{1000}$$

**$\rho_{vap}$ = 6.71524 kg/m$^3$**

## 7.2.5. Calculations for $K_V$:

There are two methods to find out the value of Kv.

1. By Equation
2. By Chart

$$\mathrm{F_{LV}} = \frac{mass\ flow\ rate\ of\ liquid}{mass\ flow\ rate\ of\ vapor} * \sqrt{\frac{density\ of\ vapor}{density\ of\ liquid}}$$

$$\mathrm{F_{LV}} = \frac{8553.27663}{13942.80728} * \sqrt{\frac{6.71524}{985.6116921}}$$

$$\mathbf{F_{LV} = 0.050}$$

$$\boldsymbol{K_V = e^{A+B\ ln\ (Flv)+\ Cln\ (Flv)^2\ +D\ ln(Flv)^3\ +E\ ln(Flv)^4}}$$

$$K_V = e^{-1.877478+(-0.814580)(-3)\ +\ (-0.187074)(-3)^2\ +(-0.014523)(-3)^3\ +(-0.001015)(-3)^4}$$

$$\boldsymbol{K_V = 0.44}$$

**From Appendix Chart:**

At $F_{LV}$ = 0.050 the value of $K_V = 0.42$ which is approximately equal to above value which we find out from equation;

### 7.2.6. Calculations for maximum velocity

$$V_{max} = (K_V)\sqrt{\frac{\rho_{liq} - \rho_{gas}}{\rho_{gas}}}$$

$$V_{max} = (0.44)\sqrt{\frac{985.6116921 - 6.71524}{6.71524}}$$

$$\mathbf{V_{max} = 5.31\ m/s}$$

### 7.2.7. Calculations for Volumetric flow rate:

**For Liquid:**

$$Q_L = \frac{\text{Liquid Flow rate}}{\text{Density of liquid}}$$

$$Q_L = \frac{8553.27663}{985.6116921}$$

$\mathbf{Q_L = 8.67814\ m^3/hr.}$

$\mathbf{Q_L = 2.41059 \times 10^{-3}\ m^3/sec}$

**For Gas:**

$$Q_g = \frac{\text{Gas Flow rate}}{\text{Density of Gas}}$$

$$Q_g = \frac{13942.80728}{6.71524}$$

$\mathbf{Q_g = 2076\ m^3/hr.}$

$\mathbf{Q_g = 0.576748\ m^3/sec}$

### 7.2.8. Calculations of Area:

$$\text{Area} = \frac{volumetric\ flow\ rate\ of\ \text{gas}}{maximum\ velocity}$$

$$\text{Area} = \frac{0.576748}{5.31}$$

$\mathbf{Area = 0.1086\ m^2}$

### 7.2.9. Calculations of Diameter

$$D = \sqrt{\frac{4\ * \text{Area}}{\pi}}$$

$$D = \sqrt{\frac{4\ * 0.1086}{3.14}}$$

$\mathbf{D = 0.37186\ m}$

### 7.2.10. Calculations of L/D ratio:

L/D Ratio for vertical flash Drum/Separator = 4 - 6

Assume L/D = 4 for verification

L/D = 4

$\frac{L}{D} = 4$

$\frac{L}{0.37186} = 4$

L = 4 * 0.37186

**L = 1.48744**

Now put value of L

$\frac{L}{D} = \frac{1.48744}{0.37186}$

$\frac{L}{D} = \ 4$

### 7.2.11. Vapor Height Calculations:

$H_v$ = 1.5D+0.45

$H_v$ = 1.5(0.37186) + 0.45

$H_v$ = 1.007 m

## 7.2.12. Liquid Height Calculations:

$$\mathrm{H_L} = \frac{4\ \mathrm{V}}{\pi\ D^2}$$

$$\mathbf{H_L} = \frac{\mathbf{V\ \ 4}}{\boldsymbol{\pi}\ \boldsymbol{D^2}}$$

**Volume Calculations:**

$V = Q_L * t$

$V = 2.41059 \times 10^{-3} * 60$ sec

## $\mathbf{V = 0.1446\ m^3}$

Whereas,

$Q_L$=height of liquid

t = Retention time

$$\mathrm{H_L} = \frac{\mathrm{V} \ * \ 4}{\pi \ * D^2}$$

$$\mathrm{H_L} = \frac{0.144635 \ * \ 4}{\pi \ * 0.37186^2}$$

**$\mathbf{H_L = 1.33243\ m}$**

## 7.2.13. Total Height Calculations:

Total height = Height of Liq + Height of Vapors

$H = H_L + HV$

$H = 1.33243 + 1.007$

## Total height = H = 2.3394 m

## 7.2.14. L/D ratio calculations:

L/D = 2.3394 /0.37186

**L/D = 6.01**

## 7.2.15. Mechanical Design

**Shell thickness ($T_S$)**

Ts =Pri/SEj-0.6P +Cc

Design Pressure; $P_d = 1.1*P_o$ (here $P_o$=Operating pressure)

=111.43 KPa

S= 79300kPa

Cc= 3mm= .003m; Ej=Joint Efficiency =0.85

Ts = (111.43) (0.2378m)/ (79300) (0.85) -(0.6) (111.43) + 0.003

Ts = 0.0033m

**Head Selection**

There are two types of Head:

1. Tori spherical (for P<1134.97KPa)
2. Ellipsoidal (for P>1134.97KPa)
3. Hemispherical for very high pressures

According to my range of pressure I am using tori spherical.

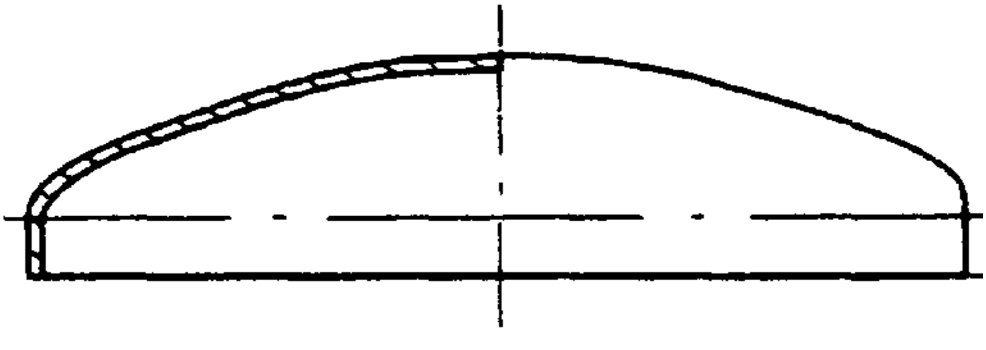


**Figure 11:** Tori spherical Shape

**Head Thickness**

Head Factor:

$X_h = 1.104*P_d/(2ES-0.2P_d)$

= (1.104*111.43)/ (2*.085*79300-0.2*111.43)

= 0.00091)

**Head Thickness:**

$T_h = X_h * D + t_c$

$= 0.00091*0.4756+0.003$

$= 0.0034m$

**Support**

These types of supports are available:

- Saddle support
- Skirt support
- Bracket support

For horizontal vessels, skirt supports, extremely tall vessels, and all other types of vessels, bracket supports are employed. For the supports of our cylindrical and vertical vessels, we will employ brackets.

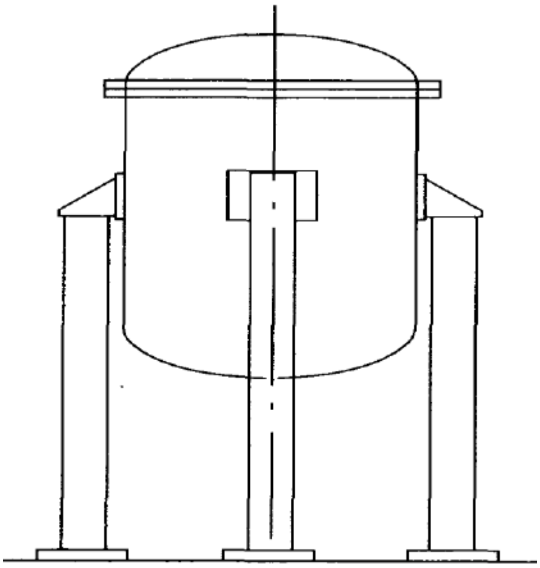


**Figure 12:** Bracket Support

## 7.2.16. Specification Sheet:

**Table 24:** Specification of Separator

| | |
|---|---|
| **Maximum Velocity** | 5.31 m/s |
| **Area** | 0.1086 $m^2$ |
| **Diameter** | 0.37186 m |
| **Total Height** | 2.3394 m |
| **Volume** | 0.1446 $m^3$ |
| **L/D Ratio** | 6.01 |

## 7.3. Absorber/Absorption Column:

### 7.4.1. Types of Absorption:

**Table 25:** Types of Absorption

| Physical Absorption | Chemical Absorption |
|---|---|
| Weak van der Waals forces are operating | The forces operating are similar to chemical bonding, but they are weaker |
| Reversible process | Irreversible Process |
| Attained equilibrium speedily | Attained Equilibrium slowly |
| Not Specific | Highly specific |

### 7.4.2. Selection of Absorbent:

The process solution is chosen based on the pressure and temperature of the gas, its composition, and the purity requirements of the treated gas.

### 7.4.3. Selection of Column type:

**Table 26:** Selection of Absorption column

| Packed Column | Plate Column |
|---|---|
| Allows vapor and liquid to mix continuously | Plate columns contact vapor and liquid in stages. |
| Packed columns have lower pressure drop | Frictional losses occur when vapor flows through liquid on each tray |
| Liquid flows in thin film in packed tower to reduce pressure drop | Plate columns require a large liquid inventory |
| Packed columns are more cost-effective and require less maintenance for corrosive liquids | For corrosive fluids, plate column is usually avoided |
| Small space requirement**.** | Relatively large in size and expensive. |

### 7.4.4. Design Parameters:

## Column design steps:

- Number of Theoretical stages
- Number of Actual stages
- Efficiency
- Diameter of column
- Height of column

## Tray design steps:

- Down comer area, net & active area
- Weir dimensions
- Hole area & number of holes
- Minimum vapor velocity
- Flooding
- Entrainment
- Pressure drops

## Number of Theoretical stages:

Number of theoretical stages will be calculating from **KREMSER method**: First of all, we have to calculate absorption factor:

$$\textbf{Absorption factor = (A) = } \frac{L}{K*V}$$

For K-Value:

| Component | Vapor Pressure | Total Pressure | K-Value |
|---|---|---|---|
| $CH_3COOH$ | 0.0458 Bar | 8.825 Bar | 0.00518 |

Table 7. 1: No. of Theoretical Stages

**Liquid Flow-rate= L= $L_{min}$ *1.5 = 3.1491 Kmol/hr.**

**Vapor Flow-rate= V = 405.2907 Kmol/hr.**

$$\text{Absorption factor = (A) = } \frac{3.1491}{0.00518*305.29}$$

$$\mathbf{A = 1.199}$$

Now, number of theoretical stages using absorption factor that comes out from equation

$$\textbf{Fraction of Solute Absorbed} = (A^{n+1} - A)/(A^{n+1} - 1)$$

Fraction of solute absorber = 1 (assuming that all solute coming in process stream is being absorbed in water or absorbent)

$$1 = (1.199^{n+1} - 1.199)/(1.199^{n+1} - 1)$$

**No. of Theoretical stages = 16.23**

## Efficiency of Column:

Density of Liquid Stream = $\rho L$ = 64.2133 lb/ft$^3$ Molecular weight of liquid stream = $M_L$ = 60

Viscosity of Solvent (Liquid Stream) = $\mu L$ = 9.11 cp

K value of desired components = 0.00518

| Components | Mole Fraction | Viscosities |
|---|---|---|
| Acetic Acid | 100% | 9.11 cp |

$$\text{Factor} = \frac{Ki*M1*\mu L}{\rho L}$$

**Factor = 0.04409**

**Efficiency = 0.90 = 90%**

**No. of Actual Stages:**

From overall stage efficiency:

$\mathbf{E_0 = N_t/N_0}$

Na = 16.23/0.90

**Na = 18**

## Entrainment flooding capacity in a Tray column:

Liquid Flow-rate = L = 3.1491 Kmol/hr.

Vapor Flow-rate = V = 408.6857

Kmol/hr. Density of Liquid = $\rho_L$ = 64.2133 lb/ft$^3$ Density of Vapor = $\rho_V$ = 50.78 lb/ft$^3$

Molecular weight of liquid = $M_L$ = 60

Molecular weights of vapor = $M_V$ = 34.047

$$FLV = \left(\frac{L}{V}\right)\left(\frac{ML}{MV}\right)\left(\frac{\rho V}{\rho L}\right)^{0.5}$$

$$\mathbf{F_{LV} = 0.012075}$$

## Diameter of Column:

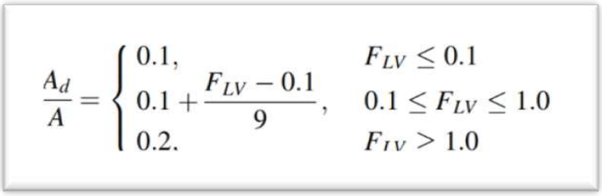
Vapor Flow-rate =V = 408.6857 Kmol/hr.

Molecular weight of vapor = $M_V$ = 34.04781 Fraction of flooding = f = 0.85

$A_d$/A taken as 0.1 on the basis of $F_{LV}$ Value

while equation used for calculating diameter is given as:

$$\mathbf{Dc} = \frac{4 * V * Mv}{f * Uf * \pi * \left(1 - \frac{Ad}{A}\right) * \rho v}$$



$$\frac{A_d}{A} = \begin{cases} 0.1, & F_{LV} \leq 0.1 \\ 0.1 + \frac{F_{LV} - 0.1}{9}, & 0.1 \leq F_{LV} \leq 1.0 \\ 0.2. & F_{IV} > 1.0 \end{cases}$$

Density of vapor = $\rho_V$ = 50.78 lb/ft$^3$

Flooding Velocity= $U_f$ = C $\left(\frac{\rho L - \rho V}{\rho V}\right)$^0.5

**$U_f$ = 29.98 ft/sec**

Actual velocity = $V_f$ = 0.75*0.8 ft/sec = 0.232 ft/sec (80% of flooding velocity).

Diameter = $D_C$ = 11.70 ft = 3.56 m

## Height of Absorber:

Height of absorption column = HC = plate spacing * Number of actual plates

## Column Height = 36ft

Height of absorption column = HC = 36 ft + 4 ft (above the tray for the removal of entrained liquid)

## HC = 40 ft

Height of absorption column = HC = 40 ft + 10 ft
(Below the bottom tray for bottom surge capacity)

**HC = 50 ft = 15.243 m**

**Area of Column:**

Area of column can be calculated as:

$$\mathbf{Ac} = \boldsymbol{\pi}\frac{\boldsymbol{D^2}}{\mathbf{4}}$$

## $A_C$=2.487 $m^2$

Down comer area can be calculated from equation bellow:

$$A_d = 12\% * A_c$$

$$\mathbf{A_d = 0.29\ m^2}$$

**Net Area:**

Net area can be calculated from equation bellow:

$$A_n = A_c – A_d$$

$$A_n = 1.587\ m^2$$

**Active Area:**

Active area can be calculated from equation bellow:

$$Aa = A_C – 2Ad$$

$$Aa = 1.907\ m^2$$

**Hole Area:**

Hole area can be calculated from equation below:

$$A_h = 10\% * A_a$$

$$A_h = 0.1907\ m^2$$

## Number of Holes:

For calculating number of holes in plates we have to take some assumptions:

Tray Spacing = $L_t$ = 0.6 m

Hole Pitch = $l_p = 3*d_h = 3*0.005 = 0.015$ m or 15 mm

Tray

Thickness = $T_t$ = 5 mm or 0.005 m

Hole size = $d_h$ = 5 mm or 0.005 m

Total Active Holes = $n_t = \frac{Total\ Hole\ Area}{Area\ of\ One\ hole}$

$$\mathbf{N_t = 9717.707}$$

## Friction for vapor flow through dry tray perforation:

$C_0$ = 0.78 (ratio of tray thickness to hole diameter)

Density of vapor = $\rho_V$ = 813.417 kg/m$^3$

Density of liquid = $\rho_L$ = 1028.59 kg/m$^3$

Hole velocity = $U_0$ = 0.232 ft/sec (80% of Flooding velocity)

$$\mathbf{Hd = 0.186*} \left(\frac{\mu 0^2}{C0^2}\right)\left(\frac{\rho v}{\rho L}\right)$$

$$\mathbf{Hd = 1.310*10^{-2}\ inch\ of\ water}$$

## Hold up of equivalent clear liquid on the try (hi):

Weir height = $h_w$ = 2 inch

Weir length = $L_W$ = 73% of $D_C$=

140.436inch Liquid flow rate = $q_L$ =

427.95 gal/min

Effective relative froth density (height of clear liquid /froth height) = $\phi_e$ = 0.526

$$\mathbf{Hi = \phi e + [h_w +} \left(\frac{ql}{Lw * \phi e}\right)^{0.67}]$$

$$\mathbf{Hi = 2.758\ inch\ of\ water}$$

## Loss due to Surface Tension:

Surface Tension of acetic acid at 25°C = $\sigma$ = 0.027 kg/s$^2$

Hole Diameter (max) = $D_b$ = 0.18 inch

$h_\sigma$ = 0.82 inch of water

$$\mathbf{h\sigma} = \left(\frac{6*\sigma}{g*\rho L*Db}\right)$$

Using Equation, we can calculate total pressure drop due to head:

$$h_t = 3.5793 \text{ inch of water}$$

## Weeping

For checking whether weeping is occurring in our process or not we have relation bellow:

$$h_d + h_\sigma < h_l$$

From equation we can conclude

0.821< 2.758Therefore, if the liquid level is uniform, weeping occurs.

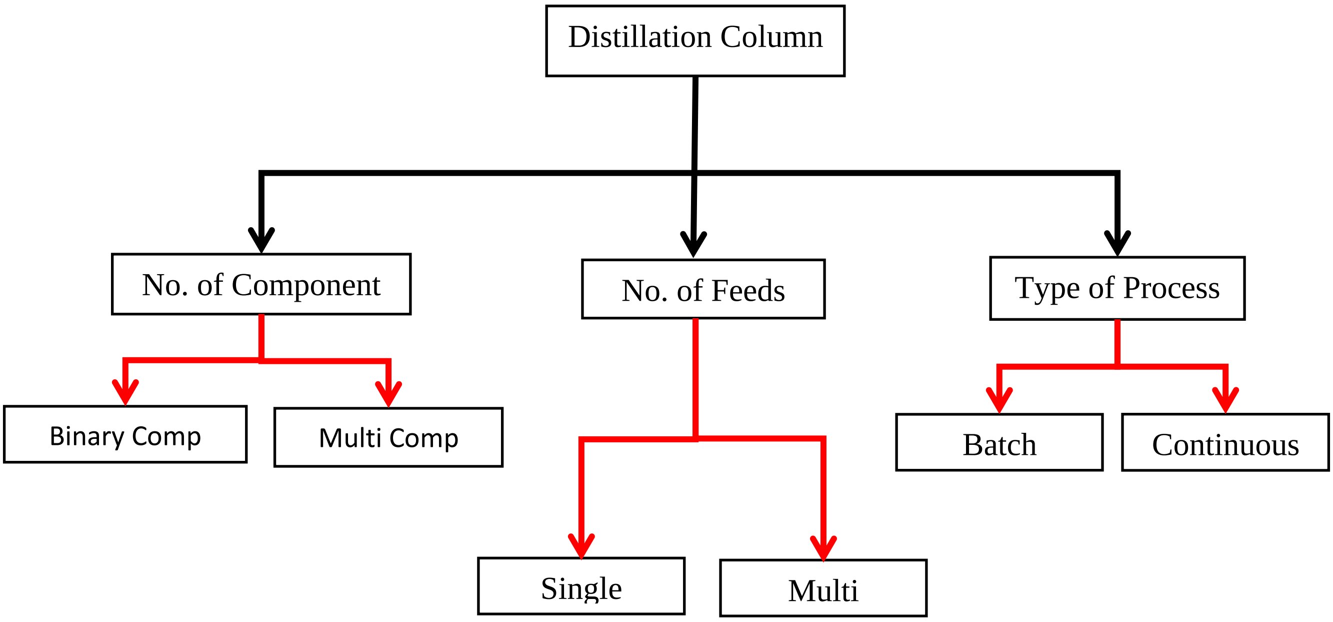
## 7.5. Distillation Column:

Distillation column is a unit operation that separates the components of a liquid mixture by boiling and condensing the mixture. The components are separated based on their different boiling points. The liquid mixture is introduced into the column and flows down due to gravity. The vapor is produced by partial vaporization of the liquid and flows up the column. The remaining liquid is withdrawn from the column as the bottom products. Here are some additional details about distillation:

- Distillation is a versatile process that can be used to separate a wide variety of liquid mixtures.
- Distillation is a commonly used process in the chemical, petrochemical, and food industries.
- Distillation can be used to separate a mixture into its individual components or to produce a purified product.

- Distillation requires a fair amount of energy. Gravity causes the liquid mixture to flow downward after being injected into the column. The liquid is partially vaporized to generate the vapor, which rises up the column. The bottom product is the liquid that is still in the column.

### 7.5.1. Classification of Distillation Column:



### 7.5.2. Types of Distillation:

Following are the top seven distillation methods:

- Steam distillation
- Extractive distillation
- Reactive distillation
- Fractional distillation
- Azeotropic distillation
- Flash distillation
- Vacuum Distillation

## 7.5.3. Selection of Distillation Column:

**Table 27:** Selection of Distillation Column

| Sr # | Distillation | Description |
|---|---|---|
| **1** | **Fractional Distillation** | Fractional distillation is a process that separates mixtures of liquids with close boiling points. The mixture is heated to a temperature at which one or more of the liquids will vaporize. The vapor is then condensed back into a liquid, and the different liquids are collected separately. Several sectors, particularly the oil and gas sector, employ fractional distillation to separate crude oil into its individual constituents, such as petrol, diesel fuel and kerosene. The chemical industry is working to separate chemical combinations like benzene and toluene. Aspirin and paracetamol are two examples of medication combinations that the pharmaceutical industry is working to separate. the facility where pure substances are prepared for study and analysis. |
| **2** | **Azeotropic Distillation** | Azeotropic distillation is a type of distillation that is used to separate mixtures that form azeotropes. An azeotrope is a mixture of two or more liquids that have the same boiling point. This means that simple distillation cannot be used to separate these mixtures, as the vapors will always contain the same proportions of the liquids as the liquid mixture itself. The third ingredient, an entrainer, is added to the mixture in azeotropic distillation to make it function. One of the components in the mixture will create an azeotrope with the entrainer, and this will cause the azeotrope to break. The combination can then undergo distillation to remove the entrainer. Many industries, particularly the petrochemical and chemical processing sectors, use azeotropic distillation. Numerous combinations, including ethanol-water, nitric acid-water, and benzene-toluene, can be separated using this technique. |
| **3** | **Extractive Distillation** | Extractive distillation is a separation process that uses a solvent to change the volatility of components in a mixture. This allows for the separation of close-boiling, pinched, or azeotropic mixtures that cannot |

| | | |
|---|---|---|
| | | be separated by simple distillation. The solvent is added to the mixture before it is distilled. The solvent interacts with the components in the mixture, changing their relative volatilities. This allows the components to be separated by distillation. Many businesses, notably the petrochemical and chemical processing sectors, use extractive distillation. Benzene-cyclohexane, ethyl acetate-ethanol, among many other mixes, are among the various mixtures that it is used to separate. |

**Table 28:** Types of Configurations

### 7.5.4. Selection of reboiler:

There are several types of reboilers used in distillation processes, including:

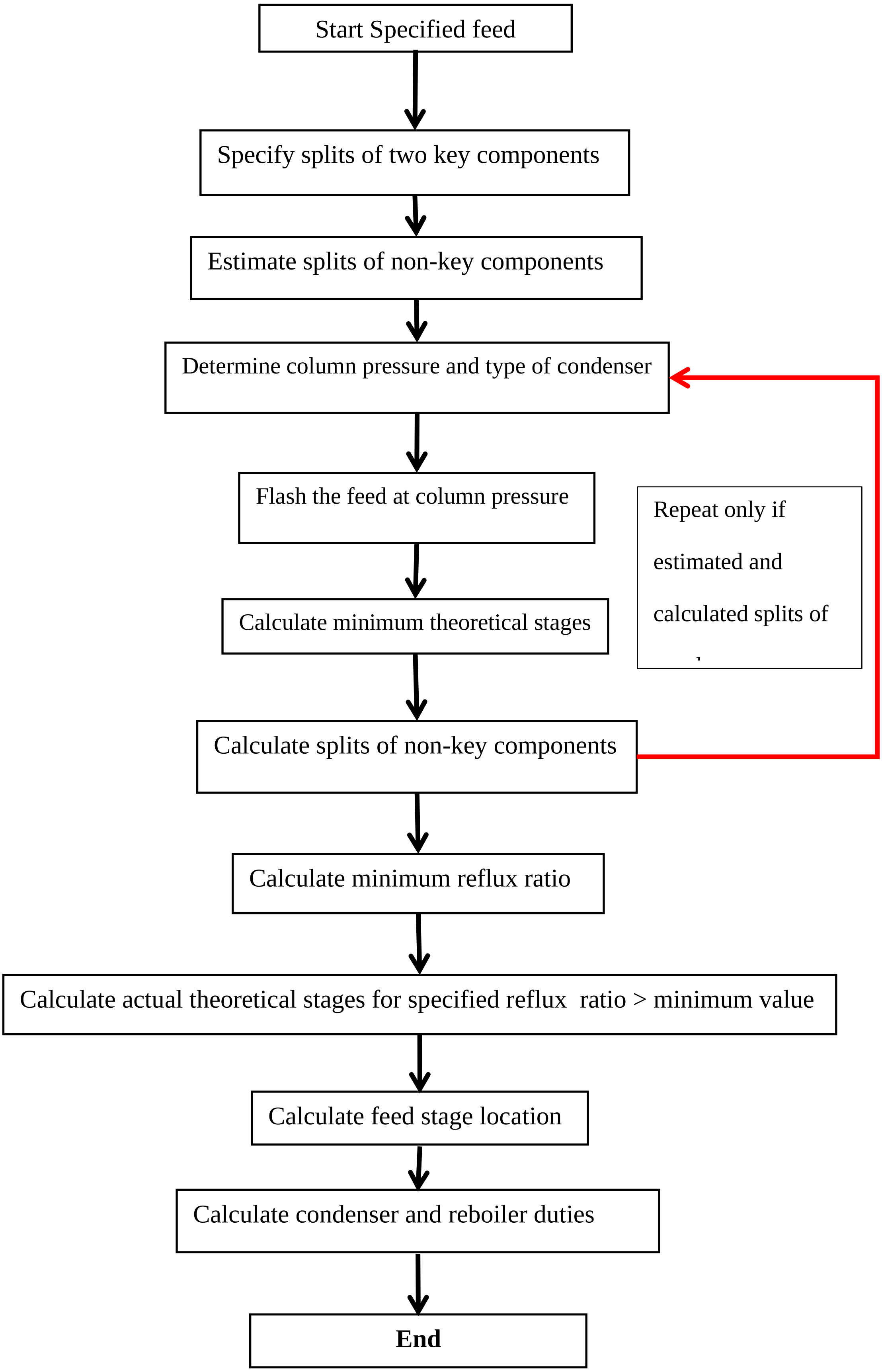
**Kettle reboilers:** These are the most common type of reboilers and consist of a shell and tube heat exchanger with a vapor-liquid separator. They are well-suited for handling large volumes of fluid and are relatively easy to maintain.

**Thermosiphon reboilers**: These use natural convection to circulate the heating medium, typically steam or hot oil, through the heat exchanger. They are often used when a large temperature difference between the heating medium and the process fluid is required.

**Forced circulation reboilers:** These use a pump to circulate the heating medium through the heat exchanger, allowing for greater control over the temperature and flow rate. Kettle reboilers are often considered the best option for several reasons.

- They are simple and reliable, with no moving parts. This makes them easy to operate and maintain.
- They have a large surface area for heat transfer, which allows for efficient operation.
- They can handle a wide range of fluid volumes and are well-suited for handling viscous fluids or those with a high solids content.
- Kettle reboilers are relatively inexpensive compared to other types of reboilers, making them a cost-effective choice.

## 7.5.5. Distillation Column Design Algorithm:



### 7.5.6. Major Design Steps:

1. Decide what the process' operational variables will be.
2. Apply the Fenske equation to get the minimal quantity of plates necessary.
3. Employ the Underwood equation to calculate the minimal reflux ratio.
4. Based on design factors, choose the theoretical reflux ratio.
5. Utilize the Gilliland correlation approach to ascertain the quantity of trays.
6. Apply the Kirkbride empirical equation to choose the best placement for the feed stage.
7. Identify the column's main measurements, such as its diameter and height.
8. Create the column's internal components.

### 7.5.7. Process Design:

#### Classification of Components:

A series of empirical equations known as the Antoine data can be used to determine the saturation vapor pressure of a liquid at a specific temperature. The relative volatility of the components in a liquid combination is commonly determined using the Antoine equations.

How readily a component can be separated from other components in a combination is determined by its relative volatility. A component can be easily isolated from other components if its relative volatility is significant. A component is difficult to isolate from other components if its relative volatility is low.

#### Reflux Ratio:

Reflux is the fraction of condensed vapor that is sent back to the top of a distillation column in order to boost productivity and stop volatile components from being lost. Depending on the reflux ratio employed, a particular separation may take one or more phases.

$$R = \frac{Flow\ returned\ as\ reflux}{flow\ of\ top\ product\ taken\ off}$$

**Relative Volatilities:**

The relative volatility of two components can be expressed as the given ratio:

$$\alpha = \frac{Vapour\ Pressure\ of\ more\ volatile\ Component}{Vapour\ Pressure\ of\ less\ volatile\ Component}$$

$$\alpha = \frac{P_A^{sat}}{P_B^{sat}}$$

**Vapor Pressure:**

The vapor pressure of a liquid can be estimated at intermediate temperatures by drawing a straight line between the critical point and the normal boiling point on a log-pressure versus reciprocal absolute temperature plot. Numerous equations have been developed to describe this relationship

One widely used equation is the three-term Antoine equation, introduced by Antoine in 1888.

$$ln\ P = A - \frac{B}{T + C}$$

where

P = vapor pressure, mmHg,
A, B, C = the Antoine coefficients,
T = temperature, K.

| Components | α at B.P | α at D.P | α geometric mean |
|---|---|---|---|
| **Oxygen** | 4013.5622 | 280.8185 | 1061.6415 |
| **Ethylene** | 751.5126 | 86.7319 | 255.3040 |
| **Carbon dioxide** | 971.6347 | 156.1905 | 389.5640 |
| **Water** | 1.7258 | 1.8970 | 1.8093 |
| **Acetic Acid** | 1 | 1 | 1 |
| **VAM** | 5.3963 | 2.8889 | 3.9484 |

On the basis of relative volatilities components are distributed into as follows:

- Light key = Oxygen, Carbon dioxide

- Heavy Key = Acetic Acid

**Calculation of Minimum No. of Stages (*N $_{min}$*):**

By using Fenske equation:

$$\left[\frac{x_i}{x_r}\right]_d = \alpha_i^{Nm} \left[\frac{x_i}{x_r}\right]_b$$

$\left[\frac{x_i}{x_r}\right]$ = The ratio of any component's concentration to that of a reference component's concentration, with the prefixes d and b designating the distillate's tops and bottoms, respectively.

$$\mathrm{N_m} = \frac{log\ \left[\frac{x_{LK}}{x_{HK}}\right]_d * \left[\frac{x_{HK}}{x_{LK}}\right]_b}{log\ \alpha_{LK}}$$

$\mathrm{N_m}$ = minimum number of stages at total reflux

$\alpha$ = average volatility of the component i with respect to the reference component.

= mole fraction of distillate of heavy key component = 0.4312

= mole fraction of distillate of light key component = 0.02411

= mole fraction of bottom of light key component = 0.0018

= mole fraction of bottom of heavy key component = 0.9981

$\alpha_{LK}$ = volatility of light component = 1.8093

Putting values in Fenske equation,

$$\mathrm{N_m} = \frac{log\ \left[\frac{x_{LK}}{x_{HK}}\right]_d * \left[\frac{x_{HK}}{x_{LK}}\right]_b}{log\ \alpha_{LK}}$$

$$\mathrm{N_m} = \frac{3.8625}{0.2575}$$

$\mathrm{N_m}$ = 14.49 ~ 15 Stages

**Calculation of Minimum Reflux Ratio ($R_{min}$):**

This can be calculated from Underwood's method:

$$\sum \frac{\alpha_i \, x_{i,d}}{\alpha_i \; - \theta} \; = \; R_m + 1$$

$\alpha_i$ = the relative volatility of component i with respect to the reference component, usually the heavy key.

$R_m$ = minimum reflux ratio

$X_{id}$ = concentration of component i in the tops

θ = the root of the equation

θ is computed using

$$\sum \frac{\alpha_i \, x_{i,f}}{\alpha_i \; - \theta} \; = \; 1 - q$$

The value of θ must lie between the values of the relative volatility of the light and heavy key

q = depends on the feed temperature

$$\frac{\alpha_A x_{fA}}{\alpha_A - \theta} + \frac{\alpha_B x_{fB}}{\alpha_B - \theta} + \frac{\alpha_C x_{fC}}{\alpha_C - \theta} + \frac{\alpha_D x_{fD}}{\alpha_D - \theta} + \frac{\alpha_E x_{fE}}{\alpha_E - \theta} + \frac{\alpha_F x_{fF}}{\alpha_F - \theta} = 1 - q$$

where,

q = 1.36 according to feed condition

| **Components** | **Inlet (A)** | **α geometric mean** |
|---|---|---|
| | **Mol fraction** | |
| **VAM** | 0.11262777 | 1061.6415 |
| **Carbon Dioxide** | 0.016476654 | 255.3040 |
| **Oxygen** | 0.000268864 | 389.5640 |
| **Water** | 0.128438269 | 1.8093 |
| **Acetic Acid** | 0.709152039 | 1 |
| **Ethylene** | 0.033036404 | 3.9484 |
| **Sum** | 1 | |

And:

$$\frac{1061.6415(0.11262777)}{1061.6415-\theta}+\frac{255.3040(0.016476654)}{255.3040-\theta}+\frac{389.5640(0.000268864)}{389.5640-\theta}$$

$$+\frac{1.8093(0.128438269)}{1.8093-\theta}+\frac{1(0.709152039)}{1-\theta}+\frac{3.9484(0.033036404)}{3.9484-\theta}=1-1.36$$

θ = common root = 1.517

$$\frac{\alpha_A x_{dA}}{\alpha_A-\theta}+\frac{\alpha_B x_{dB}}{\alpha_B-\theta}+\frac{\alpha_C x_{dC}}{\alpha_C-\theta}+\frac{\alpha_D x_{dD}}{\alpha_D-\theta}+\frac{\alpha_E x_{dE}}{\alpha_E-\theta}+\frac{\alpha_F x_{dF}}{\alpha_F-\theta}=R_m+1$$

| **Components** | **In Distillate (B)** | **α geometric mean** |
|---|---|---|
| | **Mol fraction** | |
| **VAM** | 0.378019179 | 1061.6415 |
| **Carbon Dioxide** | 0.055281366 | 255.3040 |
| **Oxygen** | 0.000902183 | 389.5640 |
| **Water** | 0.430921793 | 1.8093 |
| **Acetic Acid** | 0.024034379 | 1 |
| **Ethylene** | 0.1108411 | 3.9484 |
| **Sum** | 1 | |

**Minimum Reflux Ratio:**

$$\frac{1061.6415(0.378019179)}{1061.6415-\ 1.517}+\frac{255.3040(0.055281366)}{255.3040-1.517}+\frac{389.5640(0.000902183)}{389.5640-1.517}$$

$$+\frac{1.8093(0.430921793)}{1.8093-1.517}+\frac{1(0.024034379)}{1-1.517}+\frac{3.9484(0.1108411)}{3.9484-1.517}=R_m+1$$

$$\mathrm{R_m}=0.586$$

**Actual Reflux ratio:**

The actual reflux ratio is calculated by multiplying the minimum reflux ratio with a factor between 1.1-1.5.

$$R_m = 1.50(R_m)$$

$$R_m = 1.50(0.586)$$

$$R = 0.879$$

**Number of trays (N):**

Gilliland Correlation:

$$\mathrm{X} = \frac{R - R_{min}}{R + 1}$$

$$\mathrm{X} = \frac{0.879 - 0.586}{0.879 + 1}$$

$$\mathbf{X = 0.1559}$$

$$\mathrm{Y} = 1 - \exp\left[\left(\frac{1 + 54.5X}{11 + 117.2X}\right)\left(\frac{\mathrm{X} - 1}{\mathrm{X}^{0.5}}\right)\right]$$

$$\mathrm{Y} = 1 - \exp\left[\left(\frac{1 + 54.5(0.1559)}{11 + 117.2(0.1559)}\right)\left(\frac{(0.1559) - 1}{(0.1559)^{0.5}}\right)\right]$$

$$\mathrm{Y} = 1 - 0.4997$$

$$\mathrm{Y} = 0.5002$$

$$\mathrm{Y} = \frac{N - N_{min}}{N + 1}$$

$$0.5002 = \frac{N - 15}{N + 1}$$

$$0.5002(N + 1) = N - 15$$

$$0.5002N + 0.5002 = N - 15$$

$$0.5002N - N = -15 - 0.5002$$

$$-0.4998\,N = -15\,.5002$$

$$N = 31.01 \sim 31$$

**Feed Plate Location:**

Kirkbride Equation is used for determination of were location of feed plate

$$\frac{N_R}{N_S} = \left[\left(\frac{x_{HK,F}}{x_{LK,F}}\right)\left(\frac{x_{LK,W}}{x_{HK,D}}\right)^2\left(\frac{W}{D}\right)\right]^{0.206}$$

Also,

$$N = N_R + N_S$$

where,

$N_R$ = number of plates in rectifying section

$N_S$ = number of plates in stripping section

$x_{HK,F}$ = Conc. of heavy key (Acetic Acid) in feed = 0.71098

$x_{LK,F}$ = Conc. of light key (water) in feed = Water = 0.12845

$x_{LK,W}$= Conc. of light key in bottom = Water = 0.0018

$x_{HK,D}$= Conc. of heavy key in top = Acetic Acid = 0.02411

D = 77.0550 Kmole/hr.

W = 184.2685 Kmole/hr.

Putting values, we calculate feed location.

$$\frac{N_R}{N_S} = \left[\left(\frac{0.71098}{0.12845}\right)\left(\frac{0.0018}{0.02411}\right)^2\left(\frac{184.2685}{77.0550}\right)\right]^{0.206}$$

$$\frac{N_R}{N_S} = 0.5845$$

$$N_R = 0.5845 * N_S$$

N= 31

Rectifying Section Plates + Striping Section Plates = Total Plates

$$N_R + N_S = 31$$

$$N_s = 31 - N_R$$

Put $N_s$ in equation

$$N_R = 0.5845 * N_S$$

$$N_R = 0.5845(31 - N_R)$$

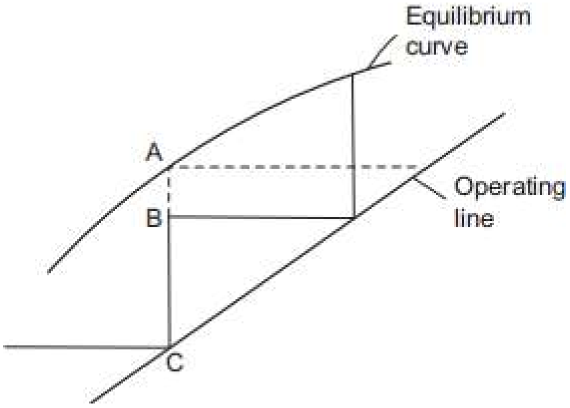
$$1.5845 N_R = 18.1195$$

$$= 11.4$$

$$\text{Feed Stage} = N_R = 11$$

### 7.5.8. Plate Efficiency:

The designer is concerned with the actual performance of a distillation column, not the idealized performance assumed in theoretical models. Equilibrium is rarely achieved in a real column, so the concept of stage efficiency is used to quantify the difference between the actual and ideal performance



$$\text{Stage efficiency} = \frac{BC}{AC} = \frac{Actual\ enrichment}{Therotical\ enrichment}$$

**Principle Definitions of efficiency:**

**Murphree plate efficiency:**

It is the ratio of the actual separation achieved to that which would be achieved in an equilibrium stage.

$$\mathrm{E_{mV}} = \frac{y_n - y_{n-1}}{y_e - y_{n-1}}$$

**Where** $y_e$ is the composition of the vapour that would be in equilibrium with the liquid leaving the plate.

**Point efficiency (Murphree point efficiency):**

If the liquid and vapor compositions are measured at a single spot on the plate, the local or point efficiency is given above. $\mathrm{E_{mv}}$

**Overall column efficiency:**

$$\mathrm{E_o} = \frac{number\ of\ ideal\ stages}{number\ of\ ideal\ stages}$$

**Methods for Prediction of plate efficiency:**

1. **O'Connell's correlation:**
2. **Van Winkle's correlation**
3. **AIChE method:**

O'Connell's correlation, however, is utilized to forecast plate efficiency since it enables quick prediction of total column efficiency.

The result of the relative volatility of the light key component (compared to the heavy key) and the overall column efficiency determines the molar average viscosity of the feed, which is computed at the average column temperature.

$$\mathrm{E_o} = 51 - 32.5 * \log(\mu_a \alpha_a)$$

$\mu_a$ = the molar average liquid viscosity, mNs/m$^2$

$\alpha_a$= average relative volatility of the light key

$\mu_a \alpha_a$ = 0.67

$\mathrm{E_o} = 51 - 32.5 * \log(0.67)$

$E_o = 56.65\%$

### 7.5.9. Plate Hydraulic Design:

### 7.5.10. Selection of Plate Contactors:

Different type of plate contactors is available some types of are given below:

1) Sieve Plate
2) Bubble cap Plate
3) Valve Plate
4) Dual Flow Plate

**Table 29:** Selection of Trays

| **Factors** | **Sieve tray** | **Valve tray** | **Bubble cap tray** | **Dual flow tray** |
|---|---|---|---|---|
| **Cost** | Low | ~1.2 times sieve trays | ~2-3 times of sieve trays | Least |
| **Capacity** | High | High | Medium high | Very high |
| **Efficiency** | High | High | High | Medium |
| **Down turn** | ~50% | ~25-30% | 10% | Least |
| **Entrainment** | Medium | Medium | High | Low to medium |
| **Total Pressure Drop** | Lowest | Medium | High | Low to medium |

| | | | | |
|---|---|---|---|---|
| **Maintenance** | Low | Low to medium | Relatively high | Low |
| **Tendency of Fouling** | Low | Low to medium | High: prone to accumulating solids | Extremely low |
| **Corrosion Effect** | Low | Low to medium | High | Very low |
| **Information for Design** | Well<br>known | Proprietarily made, but easily accessible | Well known | There is some available data. In stability, enormous diameters are possible. |

Based on the comparisons made above, "Sieve Tray Configuration" is the configuration that is most appropriate for our project.

### 7.5.11. Plate Design Procedure:

1. Key performance criteria are evaluated after a preliminary plate layout as part of the iterative plate design process. Once a good design has been produced, the design is then changed as necessary.
2. Based on the intended turn-down ratio, calculate the needed maximum and minimum vapor and liquid flow rates.
3. Identify or calculate the system's physical characteristics. Choose a starting plate spacing that will affect the overall height of the column. Typically, plate spacings between 0.15 m (6 in.) and 1 m (36 in.) are utilized, depending on the column diameter and operating conditions.
4. Calculate the column diameter taking floods into account.
5. Choose the configuration for liquid flow.

6. 6. Sketch a preliminary plate plan that indicates the weir height, the downcomer area, the active area, the hole area, and the size of the hole.
7. Evaluate the weeping rate; if it is not acceptable, go back to step 6.
8. Determine the pressure drop between the plates; if it is too great, go back to step 6.
9. Inspect the backup of the downcomer; if it is too high, go back to step 6 or step 3.
10. Specify the exact details of the plate arrangement, including the soothing zones and unperforated areas. Return to step 6 if the hole pitch is unacceptable.
11. Recalculate the flooding percentage using the chosen column diameter.
12. Determine whether the entrainment is appropriate; if it is, go back to step 4.

## Column Diameter:

$$\mathrm{F_{LV(BOTTOM)}} = \frac{L_W}{V_W}\sqrt{\frac{\rho_V}{\rho_L}}$$

$$\mathrm{F_{LV(BOTTOM)}} = 0.6241$$

$$\mathrm{F_{LV(TOP)}} = \frac{L_W}{V_W}\sqrt{\frac{\rho_V}{\rho_L}}$$

$$\mathrm{F_{LV(TOP)}} = 0.0205$$

Tray spacing = 0.30 m

*Using Fig 11.27 (Sinnott, 2005)* (

K1 (top) = 0.06

K1 (bottom) = 0.03

Correction for surface tension

**Flooding Velocity Calculation:**

Top $\mathrm{u_f} = 1.712$

$$\text{Bottom } \mathrm{u_f} = \text{Bottom k1}\sqrt{\frac{\rho_1 - \rho_v}{\rho_v}}$$

$$\text{Bottom } u_f = 0.7201$$

Design for 80% flooding at mass flow rate

$$\text{Top } u_v = 0.80 \times 1.712 = 1.3696 \frac{m}{s}$$

$$\text{Bottom } u_v = 0.80 \times 0.7201 = 0.57608 \frac{m}{s}$$

**Maximum volumetric flow rate:**

$$\text{Top } m_v = \frac{V_m}{\rho_v * 3600}$$

$$\text{Bottom } m_v = \frac{V_m}{\rho_v * 3600}$$

**Net Area:**

From Equation of Continuity we get,

or,

$$m_v = A_n V_n$$

$$\text{Top } A_n = \frac{m_v}{V_n}$$

$$\text{Top } A_n = 0.524$$

$$\text{Bottom } A_n = \frac{m_v}{V_n}$$

$$\text{Bottom } A_n = 1.247$$

**Column Cross-sectional Area:**

As First trail take downcomer area as 15% of total

$$\text{Top } \mathrm{A_c} = \frac{\mathrm{A_n}}{0.85}$$

$$\text{Top } \mathrm{u_f} = \text{Top k1} \sqrt{\frac{\rho_1 - \rho_v}{\rho_v}}$$

$$\text{Top } \mathrm{A_c} = \frac{0.524}{0.85}$$

$$\text{Top } \mathrm{A_c} = 0.6164$$

$$\text{Bottom } \mathrm{A_c} = \frac{\mathrm{m_v}}{0.85}$$

$$\text{Bottom } \mathrm{A_c} = \frac{1.247}{0.85}$$

$$\text{Bottom } \mathrm{A_c} = 1.467$$

**Column Diameter**

$$\text{Top } \mathrm{D_T} = \sqrt{\frac{4 \text{ x } A_C}{\pi}}$$

$$\text{Top } \mathrm{D_T} = \sqrt{\frac{4 \text{ x } 0.6164}{\pi}}$$

$$\text{Top } \mathrm{D_T} = 0.8859$$

$$\text{Bottom } \mathrm{D_T} = \sqrt{\frac{4 \text{ x } A_C}{\pi}}$$

$$\text{Bottom } \mathrm{D_T} = \sqrt{\frac{4 \text{ x } 1.467}{\pi}}$$

$$\text{Bottom } \mathrm{D_T} = 1.3666$$

**Liquid flow pattern:**

$$\text{Maximum volumetric liquid rate } = \frac{L'_m}{3600 * \rho_{L\,(bottom)}}$$

$$\text{Maximum volumetric liquid rate } = \frac{L'_m}{3600 * \ (x_{WATER} \text{ x } \rho_{(H2O)} + x_{A.ACID} \text{ x } \rho_{(A.ACID)})}$$

$$\text{Maximum volumetric liquid rate}$$
$$= \frac{11053.47963}{3600 * [(0.000030 \text{ x } 997) + ((0.9959 \text{ x } 1050)]}$$

$$\text{Maximum volumetric liquid rate} = \frac{11053.47963 \ kg/hr}{3600 * [(0.0307076) + (1045.8)]}$$

$$\text{Maximum volumetric liquid rate} = \frac{11053.47963}{3764990.547}$$

$$\text{Maximum volumetric liquid rate} = \ 2.9358 \text{ x } 10^{-3} \ \frac{\mathrm{m}^3}{\mathrm{sec}}$$

The liquid flow pattern is single pass because the column diameter and maximum liquid flow rate both fall within this range.

## Provisional plate design:

### i. Column Area:

$$\text{Area of cirlce } = \ \mathrm{A_C} = \frac{\pi D_C^2}{4}$$

$$\text{Area of cirlce } = \ \mathrm{A_C} = \frac{\pi * 1.3666^2}{4}$$

$$\mathrm{A_c} = 1.467 \ \mathrm{m}^2$$

### ii. Downcomer Area:

As first trial take downcomer area as 15 percent of total.

Downcomer area = $A_d$ = 0.15 x Ac

$$\mathrm{A_d} = \ 0.15 \text{ x } 1.467$$

$$\mathrm{A_d} \ = \ 0.22005 \ \mathrm{m}^2$$

### iii. Net Area:

$$A_n = A_c - A_d$$

$$A_n = 1.467 - 0.22005$$

$$A_n = 1.24695\ m^2$$

### iv. Active Area:

$$\text{Active area} = A_a = A_c - 2A_d$$

$$\text{Active area} = A_a = 1.467 - 2(0.22005)$$

$$A_a = 1.0269\ m^2$$

### v. Area of Hole:

Total hole area, Ah = 4.5 % Aa (Hole area is assumed to be 0.045 of the active area)

Total hole area = 0.045 × 1.0269 $m^2$

Total hole area = 0.04621 $m^2$

Hole diameter = $d_h$ = 2.5 mm

Plate thickness = 3 = mm

$$\text{Area of one hole} = A_h = \frac{\pi\, d_h^2}{4}$$

$$\text{Area of one holes} = A_h = \frac{\pi \text{ x } 0.0025^2}{4}$$

$$A_h = 4.90873 \text{ x } 10^{-6} m^2$$

### vi. Number of Holes:

$$\text{Number of Holes} = \frac{Total\ Hole\ Area}{Area\ of\ one\ hole}$$

$$\text{Number of Holes} = \frac{0.04621}{4.90873\ x\ 10^{-6}}$$

$$\text{Number of Holes} = 9430$$

### vii. Weir Length:

$$= \frac{A_d}{A_C} \text{x } 100$$

$$= \frac{0.22005}{1.467} \text{x } 100$$

$$\frac{L_W}{A_C} = 15$$

*From Figure*

$$\frac{L_W}{D_C} = 0.8$$

$$\text{Weir length} = L_W = 0.8 * D_C$$

$$L_W = 0.8 * 1.3666$$

$$L_W = 1.09328\, m$$

Assume then verified by iterations:

**viii. Weir height:**

Weir height = $H_w$ = 40 mm

## Check Entrainment:

$$\text{Actual Velocity} = \frac{maximum\ volumetric\ flow\ rates}{net\ area}$$

$$u_n = \frac{0.43148712}{1.24695}$$

$$\%\ \text{Flooding} = \frac{u_n}{U_f}$$

$$\%\ \text{Flooding} = \frac{0.54}{0.7201}$$

$$\%\ \text{Flooding} = 0.7498$$

$$\%\ \text{Flooding} = 75$$

$F_{LV}$ = 0.54, from figure ψ

Entrainment = Ψ = 0.0015, well below 0.1

## Check Weeping:

$$\text{Maximum liquid rate } = \frac{L_m}{3600}$$

$$\mathrm{L_w} = 6.349 \text{ kg/s}$$

Turn down ratio = 0.85

$L_{wm}$ = minimum liquid flow rate, 0.85 at turn down

$L_{wm} = 0.85\ L_w$

$L_{wm} = 0.85\ (6.349)$

$L_{wm} = 5.469$ kg/s

### Weir Crest:

Franci’s weir formula

$$\mathrm{h_{ow}} = 750\left[\frac{\mathrm{L_W}}{\rho_L * \mathrm{l_w}}\right]^{\frac{2}{3}}$$

Where,

$I_w$ = weir length, m,

$h_{ow}$ = weir crest, mm liquid,

$L_w$ = liquid flow-rate, kg/s.

$$\text{maximum } \mathrm{h_{ow}} = 750\left[\frac{\mathrm{L_W}}{\rho_L * \mathrm{l_w}}\right]^{\frac{2}{3}}$$

$$\text{maximum } \mathrm{h_{ow}} = 750\ \left[\frac{6.349}{(1045.83) * (1.09328)}\right]^{\frac{2}{3}}$$

$$\text{maximum } \mathrm{h_{ow}} = 23.5181 \text{ mm liquid}$$

$$\text{minimum } \mathrm{h_{ow}} = 750\left[\frac{\mathrm{L_{WO}}}{\rho_L * \mathrm{l_w}}\right]^{\frac{2}{3}}$$

$$\text{maximum } h_{ow} = 750 \left[\frac{5.469}{(1045.83) * (1.09328)}\right]^{\frac{2}{3}}$$

$$\text{maximum } h_{ow} = 21.29 \text{ mm liquid}$$

At minimum rate $h_w + h_{wo} = 40 \text{ mm} + 21.29 \text{ mm}$

$= 61.29$ mm liquid

Finding $K_2$ from figure 11.30 (Coulson and Richardson, Volume 6)

K2 = 30.3

The minimum design **vapor velocity**

$$u_h = \frac{[K_2 - 0.90(25.4 - d_h)]}{\rho_v^{\frac{1}{2}}}$$

$$u_h = 6.9278 \text{ m/s}$$

$$\text{Actual minimum vapor velocity} = \frac{\text{minimum vapor rate}}{A_h}$$

$V_{min}$ = Min. vapor flow rate = 0.4314 kg/s

$A_h = 0.04621 \text{ m}^2$

$$\text{Actual minimum vapor velocity} = \frac{0.4314}{0.04621}$$

$$\text{Actual minimum vapor velocity} = 9.335 \text{ m}^2$$

The weeping velocity is less than the vapor velocity, hence it is above weeping point.

**Perforated Area:**

Width of calming zones: 75 mm

Unperforated edges strip: 75 mm

$$\frac{L_W}{D_C} = 0.8$$

$\theta^0 = 109°$

Angle Held by the Plate's Edge =180° – 109° = 71°

$$\text{Unperforated Edge Strips, Average Length} = \pi \text{ x } (\mathrm{D_C} - weir\ height) \text{ x } \frac{\text{Angle at edge of plate}}{180}$$

$$\text{Unperforated Edge Strips, Average Length} = \pi \text{ x } (1.3666 - 0.075) \text{ x } \frac{109}{180}$$

$$\text{Unperforated Edge Strips, Average Length} = 2.523\text{m}$$

Area of unperforated Edge strips = $weir\ height \times Mean\ length\ edge\ strips$

$$= 0.075 \text{ x } 2.523\text{m}$$

$$= 0.1841 \text{ m}^2$$

Mean Length of Calming Zone, approximately = (Column Dia - Weir Height) * $\sin\frac{109}{2}$

$$= (1.3666 - 0.075) * (\sin\frac{109}{2})$$

$$= 1.0515 \text{ m}$$

Area of Calming Zones = 2 × (Mean length of Calming Zone × weir height)

Area of Calming Zones = 2 x 1.0515 x 0.075

Area of Calming Zones = 0.1577 m$^2$

Total Area for Perforations, Ap = Aa – Calming Zone Area – Area of Edge Strip

= 1.0269 – 0.1577 – 0.1841 = 0.6851 m$^2$

$$\frac{\mathrm{A_h}}{\mathrm{A_p}} = \frac{0.04621}{0.6851}$$

= 0.06745

$$\frac{\mathrm{I_P}}{\mathrm{d_h}} = 3.2$$

The above calculated ratio is satisfactory as it lies between the range of 2.5 – 4.0

$$\frac{\mathrm{I_P}}{\mathrm{d_h}} = 3.2$$

$$\mathrm{I_P} = 3.2 * 2.5\ \mathrm{mm}$$

$$\mathrm{I_P} = 0.008\mathrm{m\ or\ 8m}$$

**Plate Pressure Drop:**

Maximum vapor velocity through hole:

$$\mathrm{u_h} = \frac{\text{volumetric flow rate at bottom}}{\mathrm{A_h}}$$

$$\mathrm{u_h} = \frac{2.9358\ \mathrm{x}\ 10^{-3}}{0.04621}$$

$$\mathrm{u_h} = 0.0635\ \mathrm{m/s}$$

Hole diameter = $d_h$ = 2.5 mm

Plate thickness = 3 = mm

$$\frac{\text{Plate thickness}}{\text{Hole diameter}} = \frac{3}{2.5} = 1.2$$

Orifice Coefficient = $C_o$ = 0.87

**Dry plate pressure drops (hd):**

$$\mathrm{h_d} = 51 \left[\frac{\mathrm{u_h}}{\mathrm{C_o}}\right]^2 \left[\frac{\rho_\mathrm{V}}{\rho_\mathrm{L}}\right]$$

$$\mathrm{h_d} = 15.45\ \mathrm{mm\ liquid}$$

**Residual Head (hr.):**

$$\mathrm{h_r} = \frac{12.5\ \mathrm{x}10^{-3}}{\rho_\mathrm{L}}$$

$$\mathrm{h_r} = 12\ \mathrm{mm\ liquid}$$

**The total pressure drops across one plate ($h_t$):**

$$h_t = (h_{ow} + h_w) + h_d + h_r$$

$$h_t = (61.29) + 15.45 + 12$$

$$h_t = 88.74 \text{ mm liquid}$$

**Pressure drops in Pascal:**

$$\Delta Pt = 9.81 \text{ x } 10^{-3} * h_t * \rho_L$$

$$\Delta Pt = 921.36 \text{ Pa}$$

$$\Delta Pt = 0.00921 \text{ bar}$$

The pressure drop in bar is 0.00921 bar for one stage

**Overall Pressure Drop:**

$$\Delta P = \text{Acural No. of Plates x } \Delta p$$

$$\Delta P = 29 \text{ x } \Delta p$$

$$\Delta P = 31 \text{ x } 0.00921$$

Pressure drops across column

$$\Delta P = 0.28551 \text{ bar}$$

**Downcomer Liquid Backup:**

$$h_b = (h_{ow} + h_w) + h_t + h_{dc}$$

$h_b$ = Downcomer backup measured from plate surface

$h_{dc}$ = Head loss in the downcomer

The constriction at the downcomer outlet will be the primary source of flow resistance, and the equation can be used to predict head loss in the downcomer. (Coulson & Richardson Volume 6):

$$h_{dc} = 166 \text{ x } \left[\frac{L_{wd}}{\rho_L * A_{ap}}\right]^2$$

Area under the apron:

Aap = Iw × hap

So, we find $h_{ap}$;

$$h_{ap} = h_w - 10$$

$$h_{ap} = 40 - 10$$

$$h_{ap} = 30\text{mm}$$

Aap = Iw × hap

$$\text{Aap} = 1.09328\, m * 0.03\, m$$

$$A_{ap} = 0.032798\ \text{m}^2$$

Because the space beneath the apron is less than the lower area ( $\text{Ad} = 0.22005\ \text{m}^2$), so it can be used in the head loss in downcomer equation:

$$h_{dc} = 166\ \text{x}\ \left[\frac{L_{wd}}{\rho_L * A_{ap}}\right]^2$$

$$h_{dc} = 4.9\ \approx 5\ \text{mm liquid}$$

Backup in Downcomer

$$h_b = (h_{ow} + h_w) + h_t + h_{dc}$$

$$h_b = 61.29 + 88.74 + 5$$

$$h_b = 155.03\ \text{mm}$$

If hb < ½ (plate spacing + weir height) So plate spacing is acceptable

155.03 mm < ½ (300 + 40) mm

The plate spacing is acceptable as 155.03 mm < 170 mm

**Residence Time:**

$$t_r = \frac{A_d * h_{bc} * \rho_L}{L_{wd}}$$

$$t_r = \frac{A_d * h_{bc} * \rho_L}{L_{wd}}$$

$$t_r = 4.8\ \text{sec}$$

The residence time is greater than 3 seconds, hence it is feasible.

**Height of the column:**

$$\mathrm{H_C} = (\text{Number of actual plates } - 1) \times \mathrm{Hs} + (\Delta\mathrm{H})$$

Where,

Hc is the actual column height.

Nact the actual number of trays.

Hs the plate spacing.

ΔH is the additional height.

Take plate spacing as = 0.30 m

Additional height = 15% of height required by trays.

Hc = (31-1) × 0.30 + [(31-1) × 0.30× 0.15]

Hc = 10.35 m

## 7.5.12. Specification Sheet:

**Table 30:** Specification Sheet of Distillation Column

| **Identification** | | | |
|---|---|---|---|
| **Item no.** | **Equipment Name** | **Operation** | **Type** |
| **C-102** | Distillation Column | Continuous | Sieve Tray Type |
| **Function** | Separation of VAM from mixture | | |
| **Material Handled** | **Feed** | **Top** | **Bottom** |
| **Quantity** | 14681.409 kg/hr. | 3639.3907 kg/hr. | 11042.018 kg/hr. |
| **Composition of VAM** | 17.03% | 68.70% | 0% |
| **Temperature** | 34.5 °C | 75 °C | 129 °C |
| **Pressure** | 4 bars | 1.1 bar | 1.3 bar |
| **Design Data** | | | |
| **Number of Trays** | 29 | **Condenser Duty** | 1.146 MW |
| **Feed Plate located** | 11 | **Reboiler Duty** | 1.932 MW |
| **Reflux Ratio** | 0.879 | **Flooding Velocity** | 0.7201 m/sec |
| **Tray Spacing** | 0.30 m | **Tray Efficiency** | 65% |
| **Diameter** | 1.35 m | **Column Efficiency** | 56.65% |
| **Height** | 10.35 m | **Flow Arrangement** | Cross flow single pass |
| **Pressure Drop** | 0.0092 bar | | |

# Chapter 8

# Process Control & Instrumentation

## 8.1. Process Instrumentation:

For Instrumentation on various equipment's and pipeline of plants, following instrument are frequently used.

1. Temperature Sensors
2. Pressure Gauges
3. Flowmeters
4. Level measuring instruments
5. Concentration measuring instruments
6. Safety

**Objectives:**

The main objective of instrumentation and process control are:

**Safety:**

- Keep process variables within defined safe operating limits.
- To distinguish risky circumstances as they create and to give cautions and programmed shut-down frameworks.
- To e interlocks and alarms and thus prevent accidents.

**Smooth production:**

- To meet the product specifications

**Quality:**

- To ensure that the product meets the required quality standard

**Economics:**

- To work at the most minimal creation cost, in a run of the mill substance preparing plant these targets are accomplished by a blend of programmed control, manual observing and research center examination.

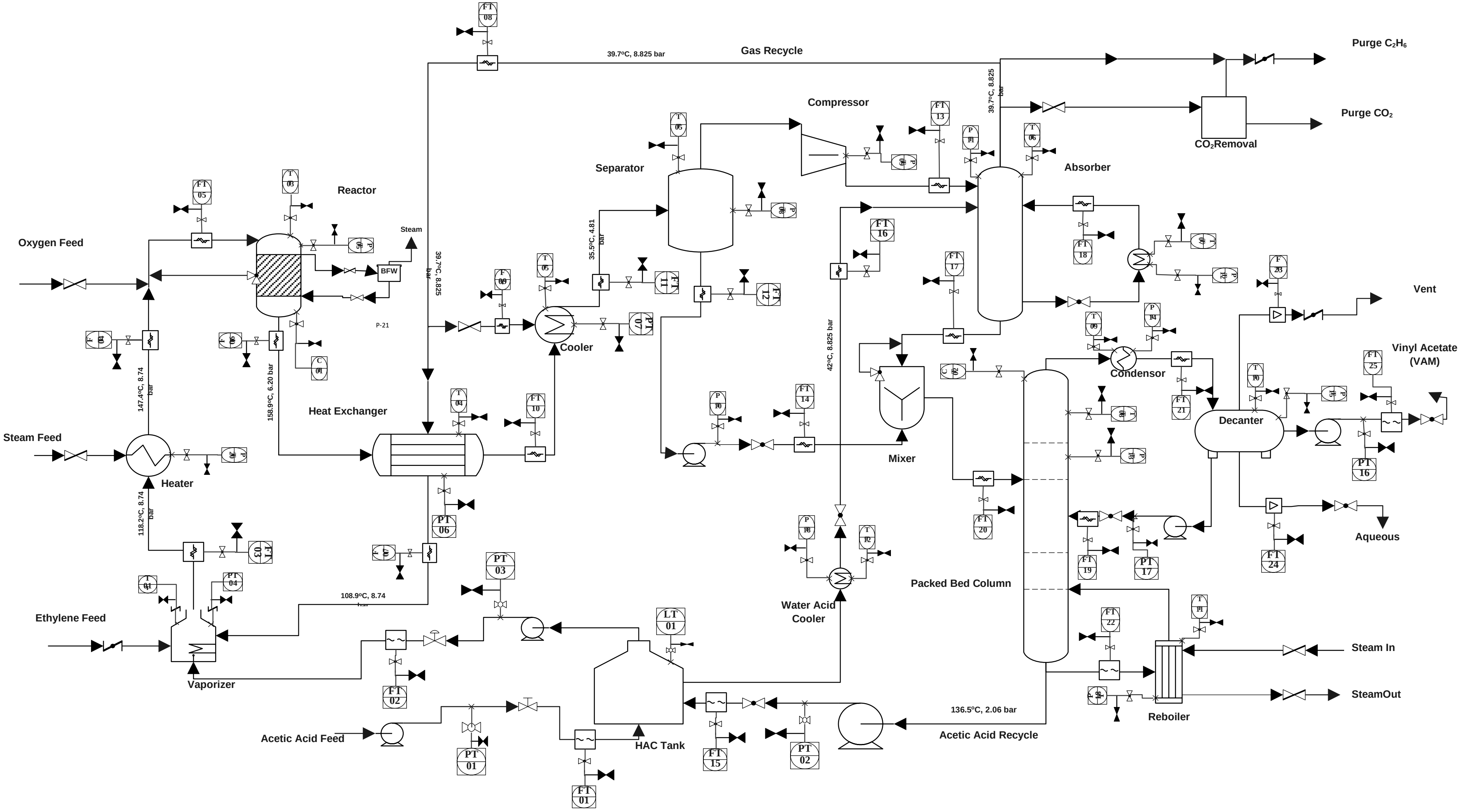


**Figure 13:** P&ID of Vinyl acetate Monomer Production

## Instrumentation On Vinyl Acetate Monomer Plant:

## Temperature Measuring Instruments:

### TT-01 to TT-11:

**Table 31:** Selected temperature measuring instruments

| Instrument Name | Reason |
|---|---|
| **RTD** | RTD with stainless steel because temp is low and stainless steel is economical.<br>RTD is robust and has liner response to temp less than 700℃.<br>RTD is widely used in industry due to its robustness and linear response |

**Table 32**: Unselected temperature measuring instruments

| Instrument Name | Reason |
|---|---|
| **Thermocouple** | **Thermocouple**: its range is high 750-1250℃ and expensive then RTD with stainless steel |
| **Pyrometer** | **Pyrometer**: NO radiation involves in our process |
| **Thermistor** | **Thermistor**: use only for lab scale. Not used in industry on equipment's |

## Pressure Measuring Instruments:

### PT-01 to PT-20:

**Table 33:** Selected temperature measuring instruments

| Instrument Name | Reason |
|---|---|
| **Pressure Differential Cell** | All pressure differential cell with isolated diaphragm because it is highly accurate, stable and rugged. |

**Table 34:** Unselected temperature measuring instruments

| Instrument Name | Reason |
|---|---|
| **Vibrating Wire** | It is sensitive. the output generated is nonlinear which can cause control problem. It cannot handle high pressure or pressure spikes. it is mostly used in lab scale |
| **Strain Gauge:** | It is not an instrument that means it cannot transmit electrical single. it is only for lab use |

## Flow Measuring Instruments:

### FT 01 to FT-02, FT-15, FT-22 TO FT-25:

**Table 35:** Selected flow measuring instruments

| Instrument Name | Reason |
|---|---|
| **Ultrasonic Flowmeter** | It is used for liquid acidic fluids. We have acetic acid so we use ultrasonic flowmeter<br>Its diaphragm is not directly in contact with acid to prevent corrosion |

**Table 36:** Unselected flow measuring instruments

| Instrument Name | Reason |
|---|---|
| **Vortex Flowmeter** | We don’t use it due to acidic medium |
| **Coriolis Flowmeter** | We don’t use it because it is expensive and use mostly for gases |
| **Electromagnetic Flowmeter** | We don’t use it because we don’t have IONS in our process |
| **Turbine Flowmeter** | We don’t use it because turbine has low flowrate accuracy. |

**FT-03 to FT-14 and FT-16 to FT-21:**

**Table 37:** Selected measuring instruments

| **Instrument Name** | **Reason** |
|---|---|
| **Coriolis Flowmeter** | It is used for mix acid and basic vapors.<br>It is best for gases and have high accuracy.<br>It is robust and most commonly used in industries |

**Table 38:** Unselected measuring instruments

| **Instrument Name** | **Reason** |
|---|---|
| **Vortex Flowmeter** | We don't use it due to acidic medium |
| **Ultrasonic Flowmeter** | We don't use it because it is suitable for acidic liquids. |
| **Electromagnetic Flowmeter** | We don't use it because we don't have IONS in our process |
| **Turbine Flowmeter** | We don't use it because turbine has low flowrate accuracy. |

**FT-23 to FT-24:**

**Table 39:** Selected measuring instruments

| **Instrument Name** | **Reason** |
|---|---|
| **Vortex Flowmeter** | It is used for liquid and gases as well at low pressure and temperature. |

**Table 40:** Unselected measuring instruments

| Instrument Name | Reason |
|---|---|
| **Coriolis Flowmeter** | We don’t use it because it is expensive and use mostly for gases |
| **Ultrasonic Flowmeter** | We don’t use it because it is suitable for acidic liquids. |
| **Electromagnetic Flowmeter** | We don’t use it because we don’t have IONS in our process |
| **Turbine Flowmeter** | We don’t use it because turbine has low flowrate accuracy. |

## Level measuring instruments:

### LT-01:

**Table 41:** Selected Level measuring instruments

| Instrument Name | Reason |
|---|---|
| **Guided Wave Radar** | Guided wave Radar are reliable and accurate level measurement instruments that require little maintenance. They have no moving parts, making them ideal for harsh environment. GWR can measure both level and interface between two media and they are not affected by media density, varying temperatures and pressures. |

**Table 42:** Unselected Level measuring instruments

| Instrument Name | Reason |
|---|---|
| **Indirect sensors-Bubble risers** | This method can be used to measure the level of corrosive liquids, the material of the tube can be chosen to be corrosion-resistant. So, the method is suitable for use in harsh environment |
| **Indirect sensors-Resistive Tapes** | The sensor is cost effective option for measuring the level of corrosive liquids or slurry. However, it is not rugged or accurate and it is prone to humidity problems. The measurement accuracy |

| | |
|---|---|
| | is also dependent on material density and sensor is not recommended for use with explosives and flammable liquids. |

## Concentration Measuring Instruments:

### CT-01 to CT-02:

Online Analyzer should be used.

A probe-based analyzer is selected as they are non-destructive and give readings in real time.

**Table 43:** Selected concentration measuring instruments

| Instrument Name | Reason |
|---|---|
| **Gas analyzer** | Gas analyzer can measure many types of components in the line. Gas analyzers work on NDIR (Nondispersive Infrared sensor). |

Offline analyzers are not allowed.

**Table 44:** Unselected concentration measuring instruments

| Instrument Name | Reason |
|---|---|
| **Spectroscopy** | Spectroscopy cannot be used as it is mostly used for discrete sampling. |
| **Gas Chromatography** | Gas chromatography can be used but it is not preferred as it destroys the sample. |
| **HPLC** | HPLC should not be used as the phase of the line is gas phase. |

## Safety:

### Relief Valve:

We use 2 relief valves:

1st relief valve is in the reactor and then it connects with the inlet stream. It is because reactor has high pressure so if there are any spikes in pressure or temperature it releases them and maintain it accordingly so no accident can happen.

2nd relief valve is in the mixer has it also has high pressure.

### Safety on instruments:

We used butt weld and then attached a globe wall. the function of globe wall is whenever our sensor is not working properly and needs to be repair, we turn off the flow by shutting globe wall and then we can easily remove the sensor and replace it

After globe wall we use Bleeder valve so if there is any backflow it releases it.

After bleeder valve our sensor/transmitter is installed.

## 8.2. Process Control

- **Control Loops:**

For instrumentation and control of various areas and gears of plants, following control circles are frequently utilized.

1. Control loop of feedback
2. Control loop of feedforward
3. Ratio control system
4. Auctioneering control system
5. Control loop of split range
6. Control loop of cascade

- **Control system elements:**

Control system has following elements:

- **Process:**

Set of operations to achieve a desired result, by specific steps is called process.

- **Computing devices:**

Every piece of framework control, estimating component is highly significant. On the off chance that estimations are not made appropriately the rest of the framework can't work acceptably, likewise the deliberate variable is picked to speak to the ideal conditions all the while.

- **Controller:**

Controller is a system which is used to regulate the process.

- **Final control element:**

The final element which controls the varying process with basic control system is called final control element.

- **Temperature Measurement & Control:**

Temperature is measured and controlled at the inlet and outlet streams of different equipment, such as coolers, heaters & heat exchanger. Different devices are used such as thermocouples, RTD etc.

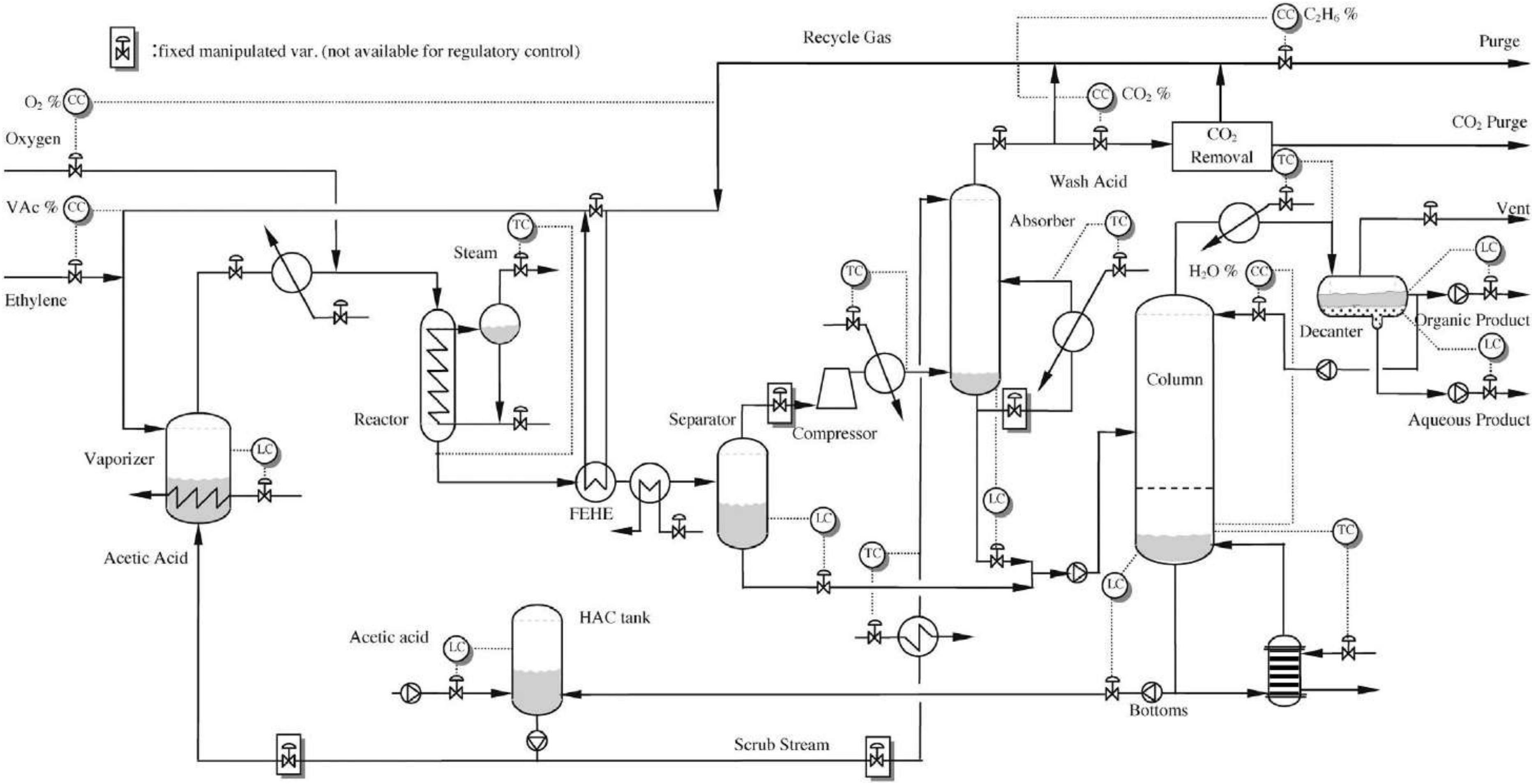


**Figure 14:** Process Control Diagram of Vinyl Acetate Monomer Production

## Reactor:

### Controlled Variables:

- Temperature inside the tubes of the reactor
- Pressure of the reactor

### Manipulated Variable:

- Flowrate of the flue gases in the shell of the reactor

### Use Loops:

### Feedback loop:

Feedback loop are also applied to the reactor, they play a crucial role in regulating the process variable. These loops constantly measure the process variable, compare it to the setpoint, and modify the control output to ensure the process variable is regulated at the desired level.

## Heat Exchanger:

### Controlled Variables:

- Temperature
- Pressure
- Product Composition

### Manipulated Variable:

- Flowrate

### Use Loops:

### Feedback loop:

Feedback loops are used to handle changing conditions dynamically. At the top of the feed inlet, we have feedback loop which are pressure transmitter transmitting the pressure to the flow indicated controller which then controls the flowrate. It is necessary to maintain the pressure of the system and feedback control loop is used.

**Cascade loop:**

- Cascade loops are also commonly used in superheater. This feature is particularly useful when there is a significant delay between control action and the effect on the mixture.
- Temperature of the outlet streams of superheater must be controlled in order to assure their correct performance and achieve the desired operating conditions in downstream or upstream process units.

## Separator:

### Controlled Variables:

- Temperature
- Pressure
- Level

### Manipulated Variable:

- Flowrate of Process fluid (inlet)
- Flowrate of Gas flowrate (product)
- Flowrate of Liquid flowrate (product)

**Use Loops:**

**Feedback Loop:**

- The level of the separator is necessary to maintain to avoid the flooding and over pressure of the separator.
- The pressure of the vessel is necessary to maintain due to safety and if the pressure is not optimal, the separation of gas and liquid can be inefficient and proper separation does not occur.
- The temperature and flow are controlled by a cascade loop. The temperature of the outlet gas is measured and sent to the temperature controller.
- The flowrate controller sends a signal to the control valve the the flowrate is changed according to the signal by the controller.

## Absorber:

### Controlled Variables:

- Pressure
- Product Composition
- Level of absorber

### Manipulated Variable:

- Flowrate

### Use Loops:

### Feedback Control:

The feedback control loop is applied in controlling the pressure of the vessel and the level of the vessel. Feedback loops respond dynamically and handle changing conditions.

### Cascade Loop:

- The **composition of the bottom** solvent is maintained by transmitting the value to the flow controller and manipulating the flowrate at the desired setpoint of the inlet gas.
- The flowrate of the inlet gas is transmitted to the flow controller.
- By taking control action earlier in the process, the cascade loop can help reduce or eliminate the impact of the delay.

## Distillation Column:

### Controlled Variables:

- Temperature at top of column
- Pressure of column
- Bottom liquid level
- Bottom temperature
- Product Composition
- Reflux ratio
- Reflux Drum Level

**Manipulated Variable:**

- Top outlet vapor flowrate
- Bottom liquid flowrate
- Feed flowrate
- Outlet flowrate of drum

**Use Loops:**

**Feedback Loop:**

To regulate the distillation column, multiple control loops are used. Feedback loops respond dynamically to changing conditions and adjust temperature, pressure, flow, and level to maintain the desired set points.

**Ratio control loop & cascade:**

A ratio control loop is a feedback control system that is designed to maintain a specific ratio between two process variables. In the case of a distillation column, the ratio control loop is used to maintain the desired reflux ratio that is 6.5 by adjusting the flow rate of either the reflux or the distillate.

**Cascade Loop:**

The temperature of the bottom is important to be maintained at 113 degrees Celsius. The reading of the bottom is transmitted to a temperature controller (primary loop) and the flow of the steam inlet of the reboiler is transmitted to the flow controller (secondary loop). The flow controller takes its setpoint from the temperature controller and the temperature setpoint is provided manually. The flow controller adjusts the steam inlet flowrate accordingly.

# Chapter 9

# Cost Estimation

## Total Capital Investment:

The total capital investment includes:

- Prime/Direct Cost
- General and Administrative/Indirect Cost.
- Fixed capital investment.
- Working capital.

## Cost Estimation:

Firstly, we find the purchased cost of every equipment in the plant.

### 9.1. Cost Estimation of the reactor:

Volume of the reactor = **10.291 $m^3$**

So, by using equation from (Towler and Sinnott second Edition):

$$C_e = a + b\,(S)^n$$

$C_e$ = Purchased cost of the equipment.

a & b= Cost constants (from Table 7.2).

S = equipment capacity.

n = exponent for that type of equipment.

So Purchased cost of the reactor is,

$$= 61500 + 32500\,(10.291)^{0.8} = \$271321.227.$$

Material factor of stainless steel (316) from Table 7.6 = 1.3

Combined cost of equipment including Purchased cost and material factor

= 1.3*271321.227

= $352717.595.

Installation factor of reactor (From Table 7.4) = 2.5.

So total cost of reactor is = 2.5*241696.3 = **$881793.989.**

## 9.2. Cost Estimation of the Heat Exchangers:

Area of the Heat exchanger is = **15.6170m$^2$**

Cost constants (from Table 7.2)

Purchased cost of Heat exchanger = $C_e$ = a + b (S)$^n$

$$= 28000 + 54\ (15.6170)^{1.2} = \$29461.204$$

Material factor of stainless steel (316) from Table 7.6 = 1.3

Combined cost of equipment including Purchased cost and material factor

= 1.3*29461.204

$ = $38299.565.

Installation factor of Heat exchanger (From Table 7.4) = 3.5

Total cost of heat exchanger = 3.5*$38299.565 = **$134048.478**

**Cost Estimation of the Flash Separator:**

Pressure in the column = 4.81 bar = 481000N/m$^2$

Length of the column = 2.3394m.

Diameter of the column = 0.37186m.

Maximum allowable stress = 1422.5*10$^5$N/m$^2$ (from Table 14.2 Towler and Sinnott second edition).

No radiography is done for welding test.

So, Efficiency is = 0.90.

Now, we find the minimum thickness of the shell so we can calculate the mass.

$$t_s = \frac{P*D}{2SE-P}$$

$$t_s = \frac{481000*0.37186}{2*1422*10^5*0.90-481000} = 0.0007\text{m} = 0.7\text{ mm}$$

Mass of column,

$$= \pi*0.0007\text{m}*0.37186*2.3394\text{m}*8000\text{kg/m}^3 = \mathbf{15.29kg}$$

Where ρ =8000kg/$m^3$ is the density of the stainless steel (304).

Purchase cost of the flash drum = 17400 + 79*$(15.29)^{0.85}$ = $1820236

Material factor for stainless steel (304) (from Table 7.6) = 1.3

Combined cost of equipment including Purchased cost and material factor = 1.3*1820236

= $23663.07.

Installation factor for column (from Table 7.4) = 4

Total cost of absorber = 4*23663.07= **$94652.3**

## 9.3. Cost Estimation of Absorber:

Pressure in the column = 4bar = 400000N/$m^2$

Length of the column = 15.243m.

Diameter of the column = 3.56m.

Maximum allowable stress = 1422.5*$10^5$N/$m^2$ (from Table 14.2 Towler and Sinnott second edition).

No radiography is done for welding test.

So, Efficiency is = 0.90.

Now, we find the minimum thickness of the shell so we can calculate the mass.

$$t_s = \frac{P*D}{2SE-P}$$

$$t_s = \frac{400000*3.56}{2*1422*10^5*0.90-400000} = 0.005572\text{m} = 5.572 \text{ mm}$$

Mass of column,

= π*0.005014m*3.56m*15.243m*8000kg/$m^3$ = **683kg**

Where ρ =8000kg/$m^3$ is the density of the stainless steel (304).

Purchase cost of the absorber = 17400 + 79*$(683)^{0.85}$ = $37671.44

Material factor for stainless steel (304) (from Table 7.6) = 1.3

Combined cost of equipment including Purchased cost and material factor = 1.3*37671.44

= \$48972.877.

Installation factor for column (from Table 7.4) = 4

Total cost of absorber = 4*48972.877= **\$195891.488**

No. of Trays = 17

Purchased cost of one tray (Sieve tray) = 130 +440*$(3.56)^{1.8}$ =\$4455.76

Purchased cost of 17 sieve trays = 17*4455.76 = \$75747.96

Material factor for stainless steel (304) (from Table 7.6) = 1.3

Combined cost of equipment including Purchased cost and material factor = 1.3*75747.96

= \$98472.351

Installation factor of Trays (From Table 7.4) = 2.5.

Total cost of Trays = 2.5*33371.481 = **\$246180.870**

**Total cost of Absorber with Trays = \$195891.488 + \$246180.870**

**= \$442072.36**

## 9.4. Cost Estimation of Multicomponent Distillation column:

Pressure in the column = 1.2 bar = 120000N/m$^2$

Diameter of the column = 1.35 m

Length of the column = 9.66 m.

No radiography is done for welding test.

Maximum allowable stress = 1422.5*10$^5$N/m$^2$ (from Table 14.2 Towler and Sinnott second edition).

So, Efficiency is = 0.56.

Now, we find the minimum thickness of the shell so we can calculate the mass.

$$t_s = \frac{P*D}{2SE-P}$$

$$t_s = \frac{120000*1.35}{2*1422*10^5*0.56.-120000} = 0.001017\text{m} = 1.017\text{mm}$$

Mass of column,

$$= \pi*0.001017m*1.35m*9.66m*8000kg/m^3 = \mathbf{333.159kg}$$

Where ρ =8000kg/m$^3$ is the density of the stainless steel (304).

Purchased cost of Multicomponent distillation column = $C_e = a + b\ (S)^n$

Cost constants (from Table 7.2)

$C_e = 17400 + 79*(333.159)^{0.85} = \$28412.3728$

Material factor for stainless steel (304) (from Table 7.6) = 1.3

Combined cost of equipment including Purchased cost and material factor = 1.3*28412.3728

= $36936.084

Installation factor for column (from Table 7.4) = 4

Total cost of Multicomponent distillation column = 4*36936.084

= **$147744.339**

No. of Trays = 29

Purchased cost of one tray (Sieve tray) = $130 + 440*(1.35)^{1.8}$ =$885.185

Purchased cost of 29 sieve trays = 29*885.185 = $25670.37

Material factor for stainless steel (304) (from Table 7.6) = 1.3

Combined cost of equipment including Purchased cost and material factor = 1.3*25670.37

= $33371.481

Installation factor of Trays (From Table 7.4) = 2.5.

Total cost of Trays = 2.5*33371.481 = **$83428.703**

Total cost of Multicomponent distillation column with Trays = $147744.339 + $83428.703

= **$231173.042**

## 9.5. Cost Estimation of Decanter:

Volume of the decanter = **10 m$^3$**

So, by using equation from (Towler and Sinnott second Edition):

$$C_e = a + b\,(S)^n$$

$C_e$ = Purchased cost of the equipment.

a & b= Cost constants (from Table 7.2).

S = equipment capacity.

n = exponent for that type of equipment.

So Purchased cost of the reactor is,

$$= 12800 + 73\,(10)^{0.85} = \$13316.80.$$

Material factor of stainless steel (316) from Table 7.6 = 1.3

Combined cost of equipment including Purchased cost and material factor

= 1.3*13316.80

= $17311.84

Installation factor of decanter (From Table 7.4) = 4.

So total cost of decanter is = 4*17238.77 = **$69247.36.**

## 9.6. Cost Estimation of Vaporizer:

Volume of the vaporizer = **17 $m^3$**

So, by using equation from (Towler and Sinnott second Edition):

$$C_e = a + b\,(S)^n$$

$C_e$ = Purchased cost of the equipment.

a & b= Cost constants (from Table 7.2).

S = equipment capacity.

n = exponent for that type of equipment.

So Purchased cost of the vaporizer is,

$$= 330+36{,}000(17)^{0.55} = \$171350.98$$

Material factor of stainless steel (316) from Table 7.6 = 1.3

Combined cost of equipment including Purchased cost and material factor

= 1.3*171350.98

= $222756.28.

Installation factor of vaporizer (From Table 7.4) = 2.

So total cost of vaporizer is = 2*17238.77 = **$445512.56.**

## 9.7. Cost Estimation of Pumps:

Purchase cost of the Pump = 8000 + 240*$(3.6)^{0.9}$ = $8760.12

Purchase cost of 5 Pumps = 5*8760.12 = $43800.6

Material factor for Aluminum and Bronze (304) (from Table 7.6) = 1.07

Combined cost of equipment including Purchased cost and material factor = 1.07*43800.6 = $46866.642.

Installation factor of Pumps (From Table 7.4) = 4

Total cost of Pumps = 4*46866.6 = **$187466.4**

## Direct Cost

Purchase equipment cost= **E = $2485966.489**

- Installation cost, 39%E = $969526.9307
- Instrumentation (installed),43%E =$1068965.59
- Piping (installed), 31%E = $770649.6116.
- Electrical (installed), 10%E = $248596.6489.
- Building (including services), 15%E =$372894.9734.
- Yard improvements, 12%E = $298315.9787.
- Service facilities (installed), 55%E = $1367281.569.

**Total Direct cost = D = $5096231.302**

## Indirect Cost

- Engineering and supervision, 32%E = \$795509.2765
- Construction expenses, 34%E = \$845228.6063
- Legal expenses, 4%E = \$99438.65956
- Contractor's fee, 19%E = \$472333.6329
- Contingency, 37%E = \$919807.6009

**Total Indirect cost = I =\$3132317.776**

## Total Capital Investment

Fixed capital investment = Direct cost + indirect cost

= \$**5096231.302** + \$**3132317.776**

**F.C.I = \$8228549.079**

Working capital 18% of F.C.I = \$1481138.834

Total Capital investment = Fixed Capital investment + Working Capital Cost.

T.C.I = \$7596477 + \$1367365.9 = **\$8963842.9**

## Product Cost:

Let us assume that fixed capital investment is depreciated using straight line method for 20 years. The salvage value at the end of plant is assumed to be 5%

Depreciation = D = $(V-V_s)/N$

Where,

V = F.C.I

$V_s$ = 0.05*F.C.I

$V_s$ = \$379823.8

N = no. of years = 20

So, **D =** \$**360832.66**

Total Product cost = Total Capital investment – Depreciation

**T.P.C = \$8603010.24.**

- Fixed charges (12% of T.P.C) = \$1032361.23

- Direct product Cost (55% of T.P.C) = $4731655.6
- Plant overhead (10% of T.P.C) = $860301.02
- Manufacturing Cost = Direct product cost + Fixed charges + plant Overhead

**Manufacturing cost = $6624317.8**

## General Expenses:

General Expenses = Administrative Cost + Distribution and selling cost + research and development cost

## Administrative Cost

It is usually 2-6% of total product cost

Administrative cost = 4% of total product cost

Administrative cost = **$344120.4**

Distribution and Selling cost:

Typically, 2-20% of the overall cost of the product goes towards distribution and marketing expenses, which include the cost of sales offices, salespeople, shipping, and advertising.

Consider the distribution and Selling cost = 12% of total product cost.

Distribution and Selling cost = **$1032361.2**

## Research and Development Cost:

It is about 5 % of total product cost.

Research and Development Cost = $430150.5.

**Financial (interest):**

It is about 0-10% of total Capital Investment.

Consider interest is 6% of total capital investment.

So, interest is = **$537830.6**

Then,

**General Expenses =$1806632.1.**

So,

Total Product cost = Manufacturing cost + General Expenses

**Total Product cost = $8430949.9**

## Gross Earing/ Income:

Wholesale selling price of VAM per ton = $1867.

Total income = selling price*quantity of product manufactured

Total income = 1867*10,000

Total income = **$18670000**

Gross income = Total income – Total product cost

Gross income = $18670000 - $8430949.9

Gross income = **$10239050.1.**

Taxes (40% of Gross income) = **$4095620.04**

Net profit = Gross income – Taxes

Net profit =$10239050.1 - $4095620.04 = **$7043430.1**

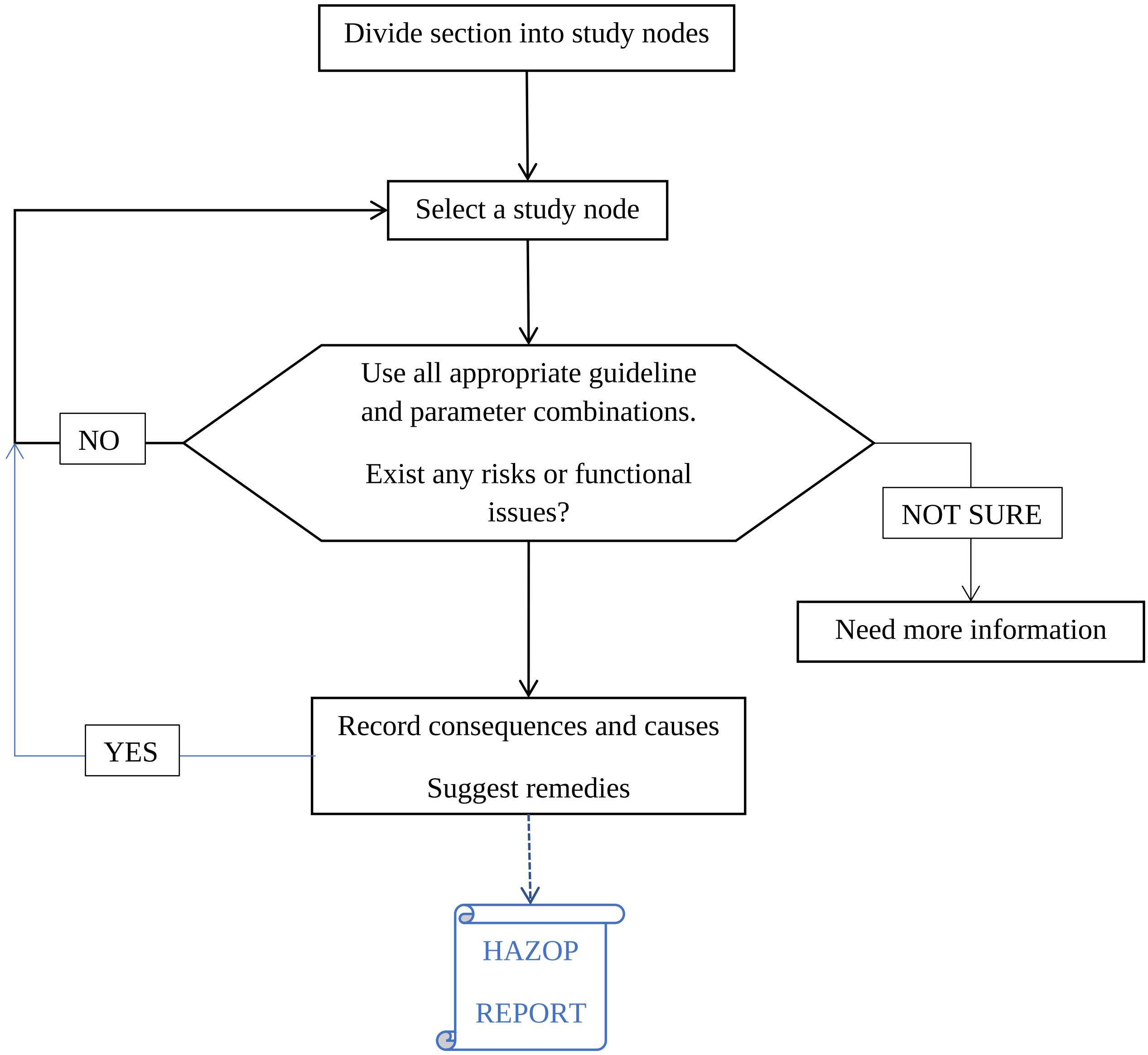
# Chapter 10

# HAZOP

## HAZOP:

HAZOP is a technique that has been developed over the past few decades to identify potential hazards and compatibility problems that may arise due to deviations from the design in both new and existing process plants. It involves conducting a systematic study to clarify the impact of deviations on the plant's processing. Often, too much emphasis is placed on identifying hazards to the detriment of potential problems. However, it is in this latter area where the benefits of a HAZOP study are usually the greatest.

## Algorithm:



## 10.1.Reactor:

**Table 45: HAZOP Study on Reactor**

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| **Flow** | | | | |
| NO | No heating | Flue gas value malfunction | Temperature decreases in reactor | Install temperature alarm (TAH) |
| REVERSE | Reverse heating flow | Failure of heating media source resulting in backward flow | Less heating, Possibility runaway reaction | Install check value |
| MORE | More cooling flow | Control valve failure, Operator fails to take action on alarm | Too much heating, off spec product and shut down of reactor/explosion | Install control valve and instruct the operators on procedure |
| AS WELL AS | Reactor product in tubes | More pressure in reactor | Off-spec product | Check maintenance procedures and schedules |
| OTHER THAN | Another material beside heating media | Water source contaminated | May be heating ineffective | If less heating, (TAH) will detect |
| **Temperature** | | | | |
| LOW | Low heating | Low heating media supply | Reaction rate slow down | Install high level alarm and instruct operators |
| HIGH | More heating | More heating media supply | Reactor may explode | Install a control valve and low-level alarm |
| **Pressure** | | | | |
| LOW | Low pressure | Partially plugged heating line | Diminished heating, Possible runaway | Install controller with maintenance |

|  |  |  |  |  |
|---|---|---|---|---|
|  |  |  |  | procedure |
| HIGH | High pressure | Control Valve fails open.<br>Controller fails and open valves | Reactor Overheat, Reaction stops<br>As above | Instruct operator and update procedure |

## 10.2.Heat Exchanger:

**Table 46:** HAZOP Study on Heat Exchanger

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| **Flow** |  |  |  |  |
| NO | Cooling fluid flow | Failure of cooling water inlet valve to closed | Process fluid temperature not lowered accordingly | Install temperature indicator before and after the process |
| MORE | Cooling water flow | Failure of cooling water inlet valve to open | Process fluid temperature too low | Install temperature indicator before and after the process |
| LESS | Cooling water flow | Pipe leakage | Process fluid temperature not lowered accordingly | Installation of flow meters |
| **Temperature** |  |  |  |  |
| LOW | Tube side temperature | High flowrate of cooling water | Process fluid temperature too low | Install (TIA) |
| HIGH | Tube side temperature | Tube side outlet valve fully opened | Tube damage, Rupture | High temperature alarm must be installed |
| **Pressure (Shell side)** |  |  |  |  |
| LOW | Shell side pressure | Pump tip | No significant effects | Not applicable |
| HIGH | Shell side pressure | Shell side discharge valve fully opened | Shell side will be over pressurized | Install high pressure alarm |
| **Pressure (Tube side)** |  |  |  |  |
| HIGH | Tube side pressure | Shell side discharge valve fully opened | Tube maybe rupture | Install high pressure alarm |

## 10.3.Flash Separator:

**Table 47:** HAZOP Study on Separator

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| **No, Not, None** | Flow | Pipe ruptures<br>Close outlet valve<br>Control valve failure | No separation occurs | Install alarm/ sensor<br>Install Automated Open & Closure of valve |
| **Less** | Flow | Valve Partially closed<br>Pipe leakage | Not Separation proceeds<br>Separator not work efficiently | Install Flowmeter |
| **More** | Flow | Failure of control valve,<br>The operator failed to take appropriate action to address the alarm | Fluid damage the diverter of separator | Install flowmeter |

## 10.4.Absorber:

**Table 48:** HAZOP Study on Absorber

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| | | **Pressure** | | |
| **HIGH** | More pressure | Gas flow high | Equipment damage & safety hazard | Install pressure gauge |
| | | **Temperature** | | |

| | | | | |
|---|---|---|---|---|
| **LOW** | Low temperature | Decreased heat input | Blockage due to heating | Increase heating capacity |
| **HIGH** | More temperature | Increased, malfunction of temperature control | Reduced efficiency of absorption | Adjust flowrate by using a controller |
| **Level** | | | | |
| **HIGH** | High liquid level | Liquid flowrate too high | Risk of equipment damage | Level control, automatic shutdown system |
| **LOW** | Low efficiency of absorption | Inadequate liquid gas contact | Reduced product quality | Modify packing and adjust flowrate |

## 10.5.Storage Tank:

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| **No, Not, None** | No Flow level | Failure of process flow inlet valves | Product offset | Installation check valves |
| **Less, Low** | More Flow level | Pump stops | Possible damage to pump | Pump shutdown automatically when level is too low |
| **More, High** | High Flow level | Failure of the level control system and pump stops | Overflow could cause. Overflow would be contained by secondary containment system | Inlet valve, level control system and pumps are inspected. There is a redundant level control system |

## 10.6.Distillation Column:

**Table 49:** HAZOP Study on Distillation Column

| Guide Word | Deviation | Causes | Consequences | Action |
|---|---|---|---|---|
| **No, Not, None** | No flow | Pipe blockage<br>Control valve failure<br>Pump Off | Column dry out<br>Possible dangerous concentration<br>No operation | Install low level alarm,<br>Check maintenance procedure and schedule |
| **Less, Low** | Less flow | Pipe leakage<br>Valve half open | Column dry out<br>Changes in product quality | Install low level alarm<br>Check maintenance procedure and schedule |
| | Low pressure | line leakage | Low efficiency of separation<br>Loss of products | Install pressure indicator |
| **More, High** | More flow | Control valve is fully opened,<br>Increase pumping capacity,<br>Control valves failure | Flooding in the column | Install high level alarm |
| | High pressure | Pressure indicator controller fail | Low efficiency of separation<br>Rupture of column or other related equipment<br>Product loss | Install high pressure alarm<br>Install pressure relief valve |
| | High temperature | High steam pressure,<br>Instrumentation failure | Separation cannot be done<br>Changes in product quality | Install temperature indicator |

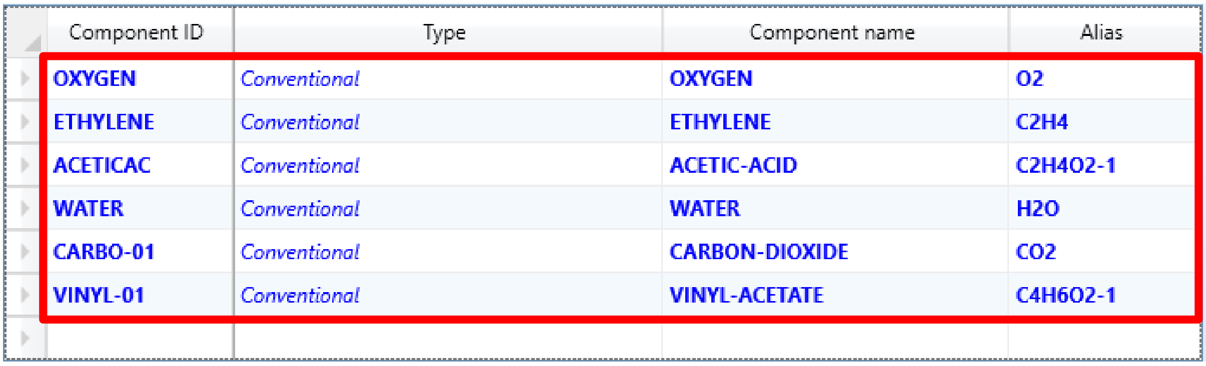
# Chapter 11

# Simulation

## 11.1.Properties:

### 11.1.1. Selected Components:

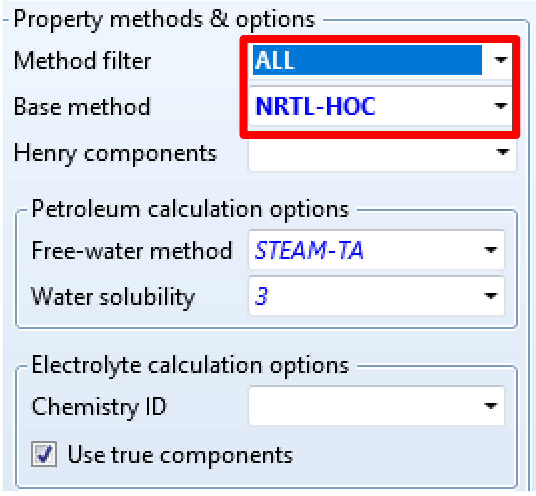
First of all, we select the components:



| Component ID | Type | Component name | Alias |
|---|---|---|---|
| OXYGEN | Conventional | OXYGEN | O2 |
| ETHYLENE | Conventional | ETHYLENE | C2H4 |
| ACETICAC | Conventional | ACETIC-ACID | C2H4O2-1 |
| WATER | Conventional | WATER | H2O |
| CARBO-01 | Conventional | CARBON-DIOXIDE | CO2 |
| VINYL-01 | Conventional | VINYL-ACETATE | C4H6O2-1 |

**Figure 15:** Selected Components

### 11.1.2. Base Method:



Property methods & options

Method filter: ALL

Base method: NRTL-HOC

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

☑ Use true components

**Figure 16:** Property Method Selection

- We use NRTL-HOC as a property package.

The decision to select the NRTL-HOC model was based on the composition of the liquid phase, which primarily consists of vinyl acetate (a polar), water (polar), and acetic acid (polar). Given that these compounds are well-known and interaction parameters are available, it was crucial to choose a model that could accurately represent their behavior. In this regard, extensive research, including consultation of the Alexandre D. Dimian book, was conducted, considering various models such as

NRTL, UNIQUAC, and their variations. Ultimately, the NRTL-HOC model was deemed the most appropriate choice to ensure precision when dealing with these specific components.

## 11.2.Simulation:

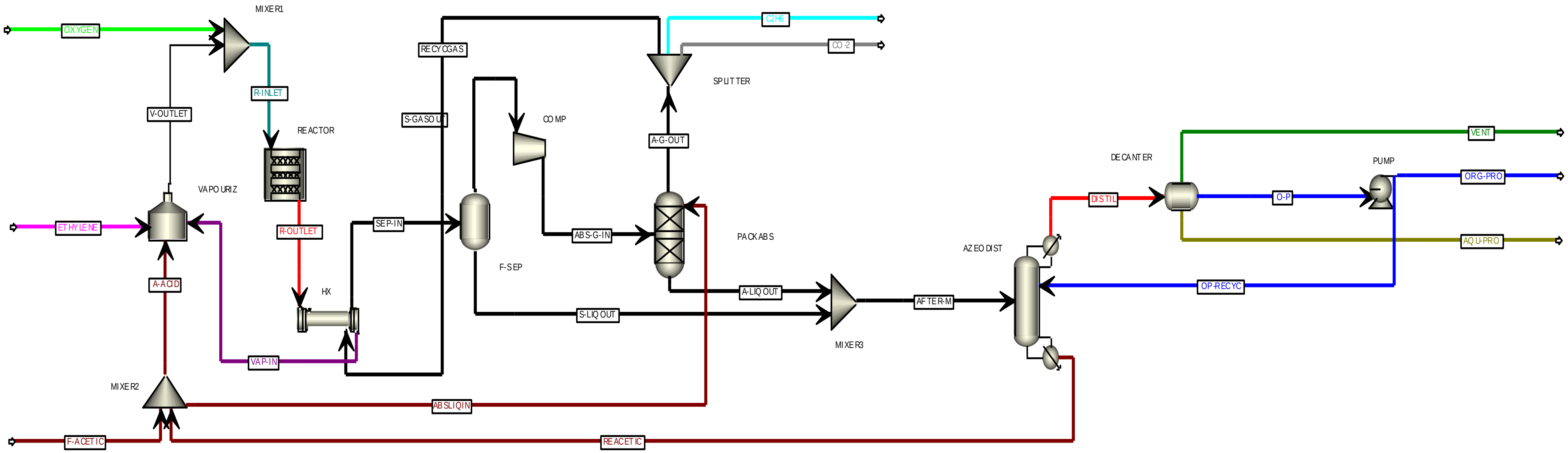
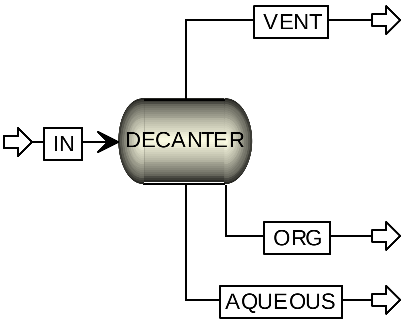
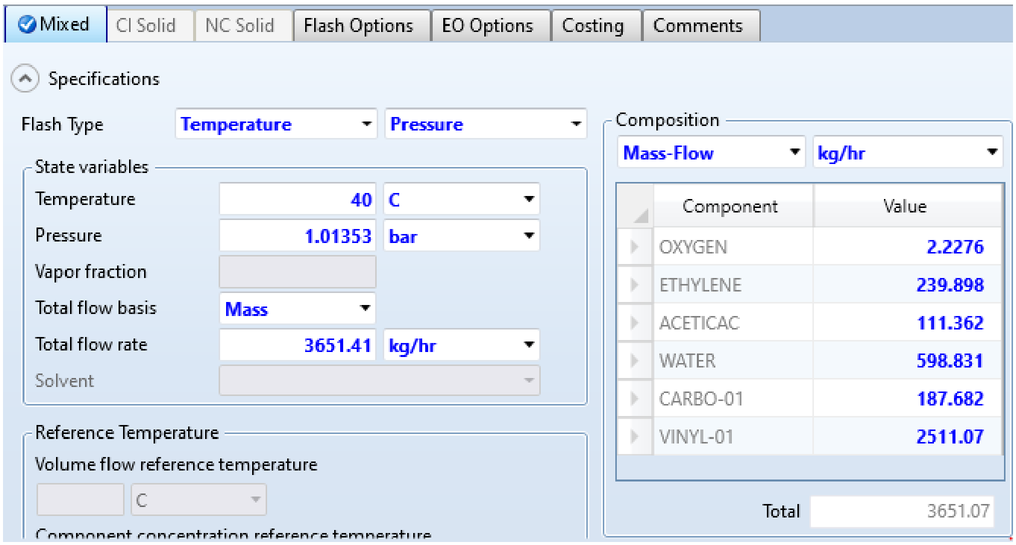


Figure 17: Flowsheet of VAM plant

### 11.2.1. Decanter:



## Feed Specifications:



Specifications

Flash Type: Temperature, Pressure

State variables
Temperature: 40 C
Pressure: 1.01353 bar
Vapor fraction:
Total flow basis: Mass
Total flow rate: 3651.41 kg/hr
Solvent:

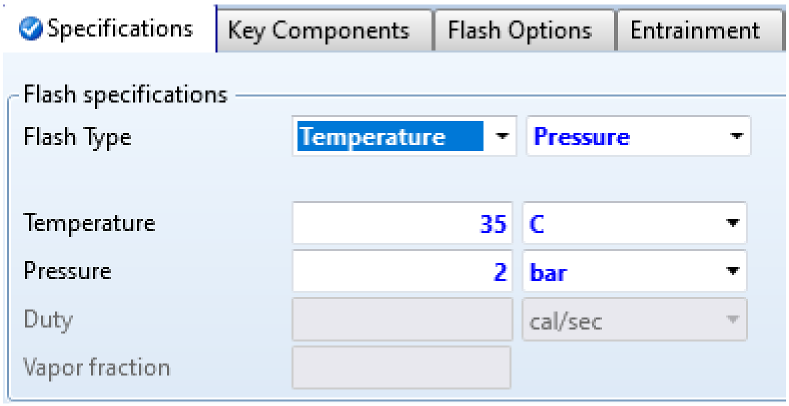
Reference Temperature
Volume flow reference temperature
C
Component concentration reference temperature

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 2.2276 |
| ETHYLENE | 239.898 |
| ACETICAC | 111.362 |
| WATER | 598.831 |
| CARBO-01 | 187.682 |
| VINYL-01 | 2511.07 |

Total: 3651.07

## Decanter Specifications:



Flash specifications

Flash Type: Temperature, Pressure

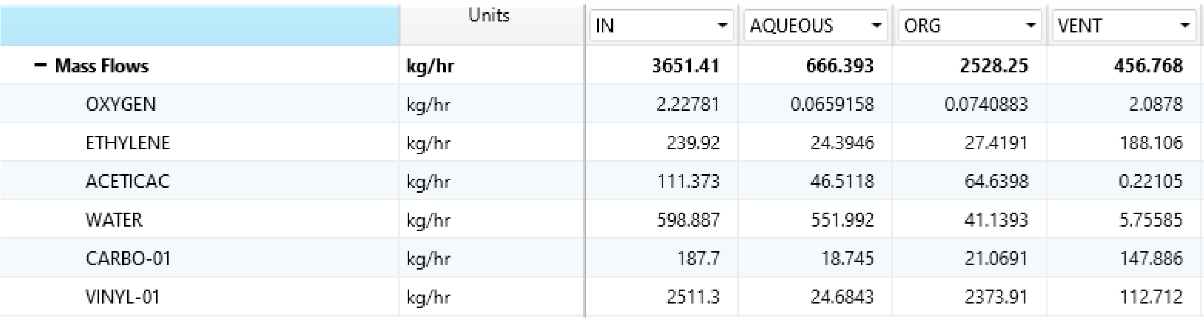
Temperature: 35 C

Pressure: 2 bar

Duty: cal/sec

Vapor fraction:

## Stream Results of Decanter:



| | Units | IN | AQUEOUS | ORG | VENT |
|---|---|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **3651.41** | **666.393** | **2528.25** | **456.768** |
| OXYGEN | kg/hr | 2.22781 | 0.0659158 | 0.0740883 | 2.0878 |
| ETHYLENE | kg/hr | 239.92 | 24.3946 | 27.4191 | 188.106 |
| ACETICAC | kg/hr | 111.373 | 46.5118 | 64.6398 | 0.22105 |
| WATER | kg/hr | 598.887 | 551.992 | 41.1393 | 5.75585 |
| CARBO-01 | kg/hr | 187.7 | 18.745 | 21.0691 | 147.886 |
| VINYL-01 | kg/hr | 2511.3 | 24.6843 | 2373.91 | 112.712 |

### 11.2.2. Separator:

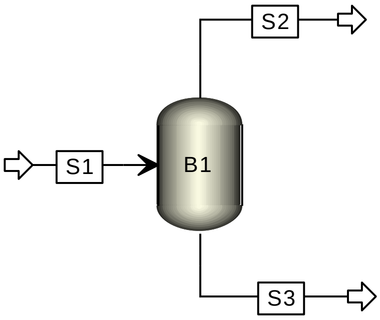
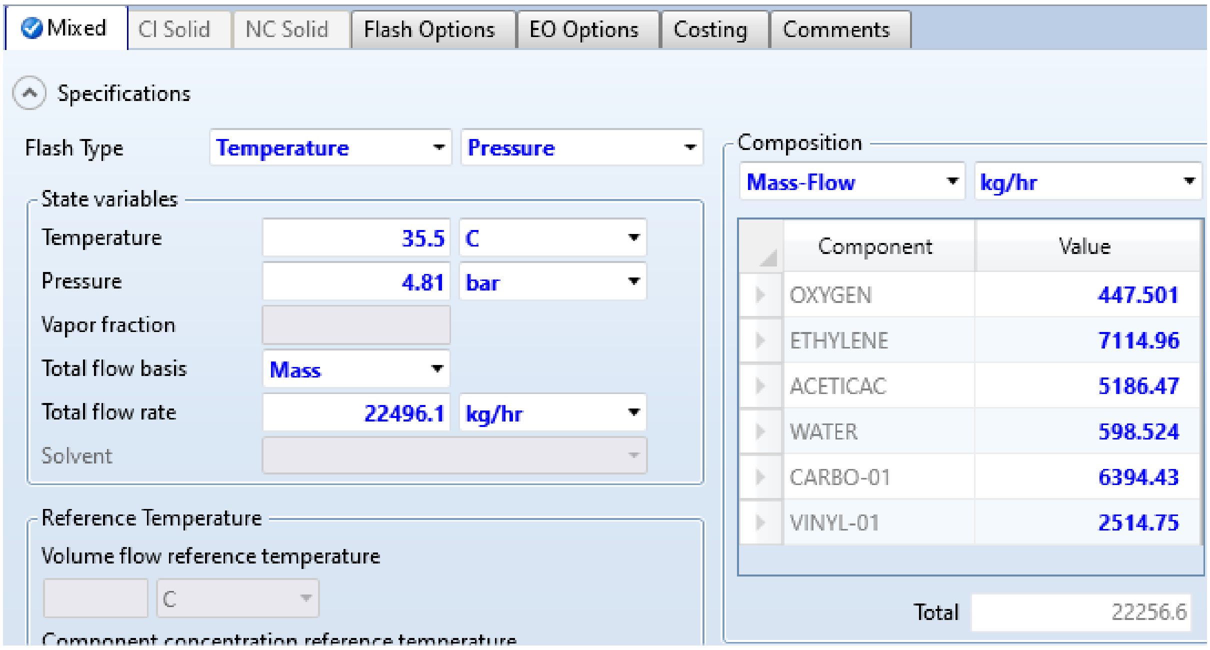


Figure 18:Simulated Figure of Separator

## Feed Specifications:



Flash Type: Temperature, Pressure

State variables

Temperature: 35.5 C

Pressure: 4.81 bar

Vapor fraction:

Total flow basis: Mass

Total flow rate: 22496.1 kg/hr

Solvent:

Reference Temperature

Volume flow reference temperature: C

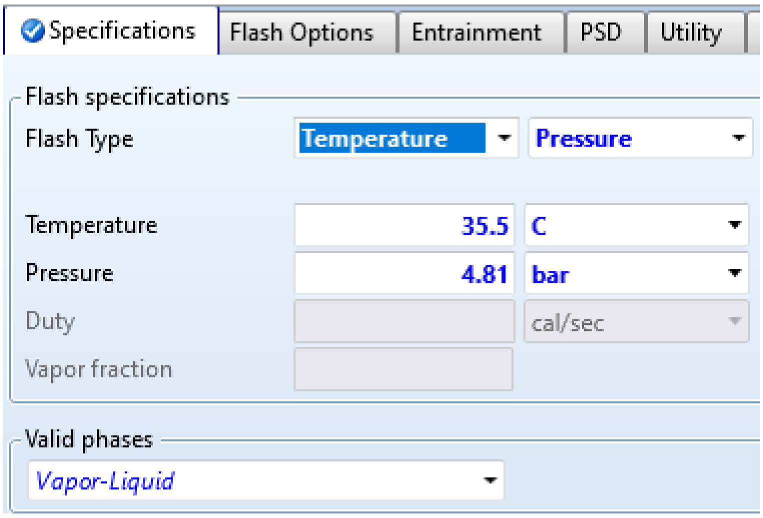
Component concentration reference temperature

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 447.501 |
| ETHYLENE | 7114.96 |
| ACETICAC | 5186.47 |
| WATER | 598.524 |
| CARBO-01 | 6394.43 |
| VINYL-01 | 2514.75 |

Total: 22256.6

## Separator Specifications:



Flash specifications

Flash Type: Temperature, Pressure

Temperature: 35.5 C

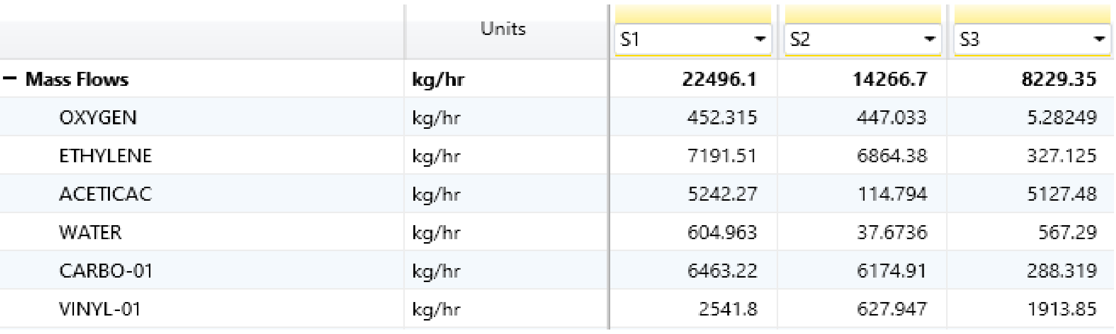
Pressure: 4.81 bar

Duty: cal/sec

Vapor fraction:

Valid phases: Vapor-Liquid

## Stream Results of Separator:



|  | Units | S1 | S2 | S3 |
|---|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **22496.1** | **14266.7** | **8229.35** |
| OXYGEN | kg/hr | 452.315 | 447.033 | 5.28249 |
| ETHYLENE | kg/hr | 7191.51 | 6864.38 | 327.125 |
| ACETICAC | kg/hr | 5242.27 | 114.794 | 5127.48 |
| WATER | kg/hr | 604.963 | 37.6736 | 567.29 |
| CARBO-01 | kg/hr | 6463.22 | 6174.91 | 288.319 |
| VINYL-01 | kg/hr | 2541.8 | 627.947 | 1913.85 |

### 11.2.3. Distillation Column:

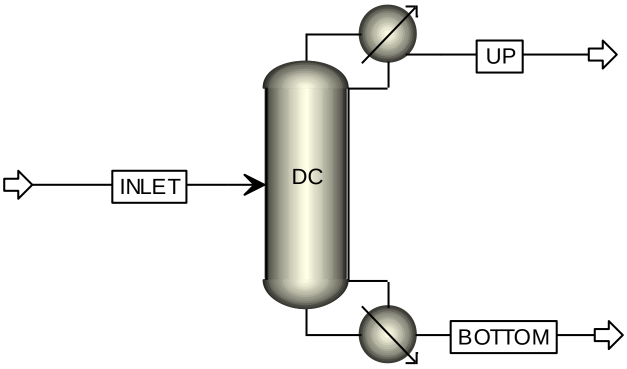
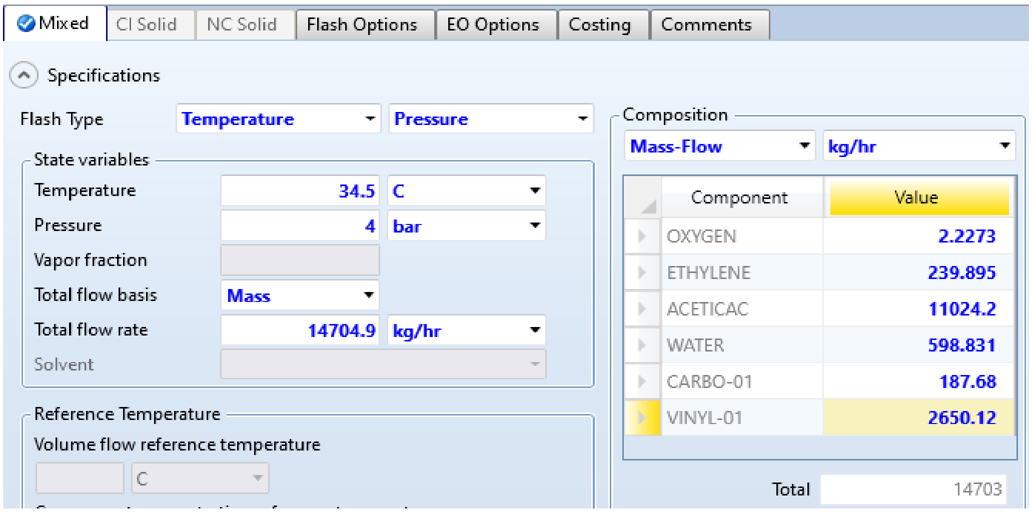


Figure 19:Simulated Figure of Distillation Column

## Feed Specifications:



Specifications

Flash Type: Temperature, Pressure

State variables

Temperature: 34.5 C

Pressure: 4 bar

Vapor fraction:

Total flow basis: Mass

Total flow rate: 14704.9 kg/hr

Solvent:

Reference Temperature

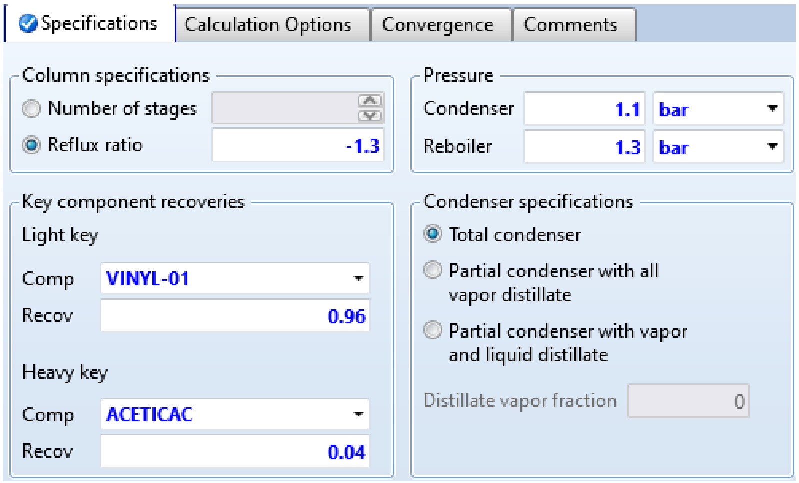
Volume flow reference temperature: C

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 2.2273 |
| ETHYLENE | 239.895 |
| ACETICAC | 11024.2 |
| WATER | 598.831 |
| CARBO-01 | 187.68 |
| VINYL-01 | 2650.12 |

Total: 14703

## Distillation Column Specifications:



Column specifications

○ Number of stages

● Reflux ratio: -1.3

Pressure

Condenser: 1.1 bar

Reboiler: 1.3 bar

Key component recoveries

Light key

Comp: VINYL-01

Recov: 0.96

Heavy key

Comp: ACETICAC

Recov: 0.04

Condenser specifications

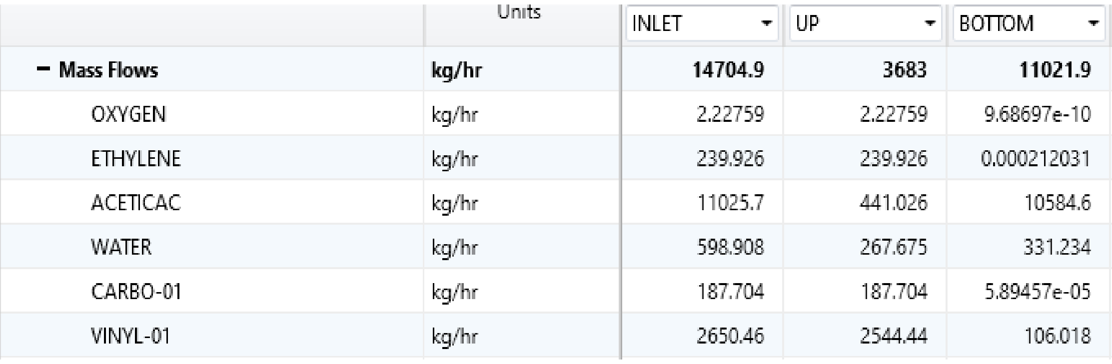
● Total condenser

○ Partial condenser with all vapor distillate

○ Partial condenser with vapor and liquid distillate

Distillate vapor fraction: 0

**Stream Results of Separator:**



| | Units | INLET | UP | BOTTOM |
|---|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **14704.9** | **3683** | **11021.9** |
| OXYGEN | kg/hr | 2.22759 | 2.22759 | 9.68697e-10 |
| ETHYLENE | kg/hr | 239.926 | 239.926 | 0.000212031 |
| ACETICAC | kg/hr | 11025.7 | 441.026 | 10584.6 |
| WATER | kg/hr | 598.908 | 267.675 | 331.234 |
| CARBO-01 | kg/hr | 187.704 | 187.704 | 5.89457e-05 |
| VINYL-01 | kg/hr | 2650.46 | 2544.44 | 106.018 |

### 11.2.4. Mixer:

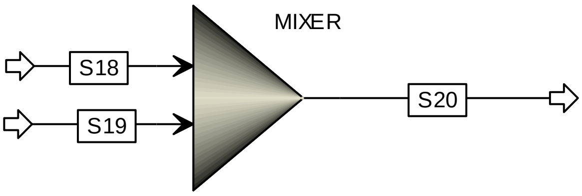
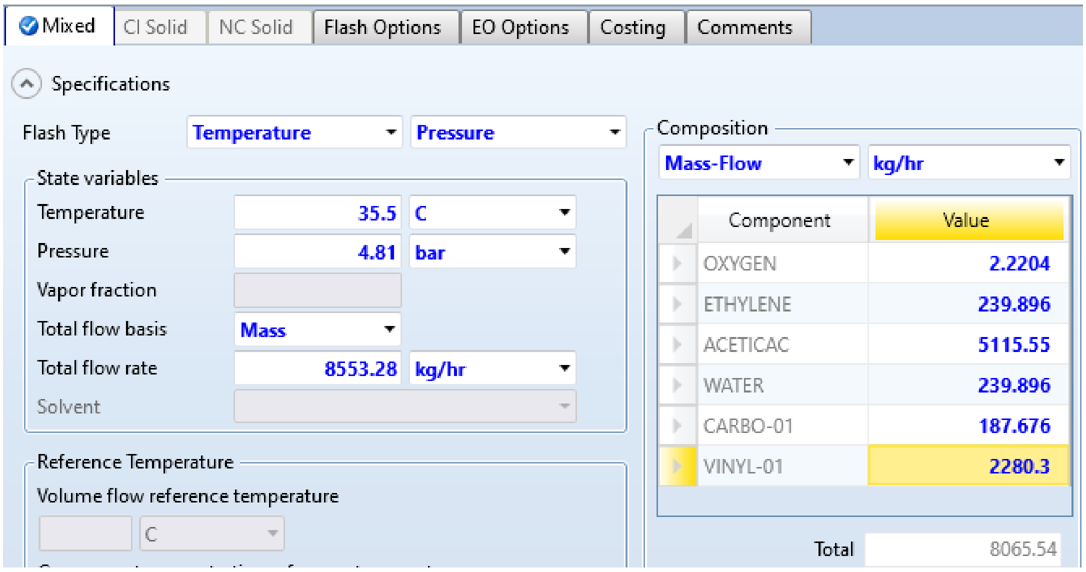


**Figure 20:** Simulated Figure of Mixer

**S18 Specifications:**



Specifications

Flash Type: Temperature, Pressure

State variables

| | | |
|---|---|---|
| Temperature | 35.5 | C |
| Pressure | 4.81 | bar |
| Vapor fraction | | |
| Total flow basis | Mass | |
| Total flow rate | 8553.28 | kg/hr |
| Solvent | | |

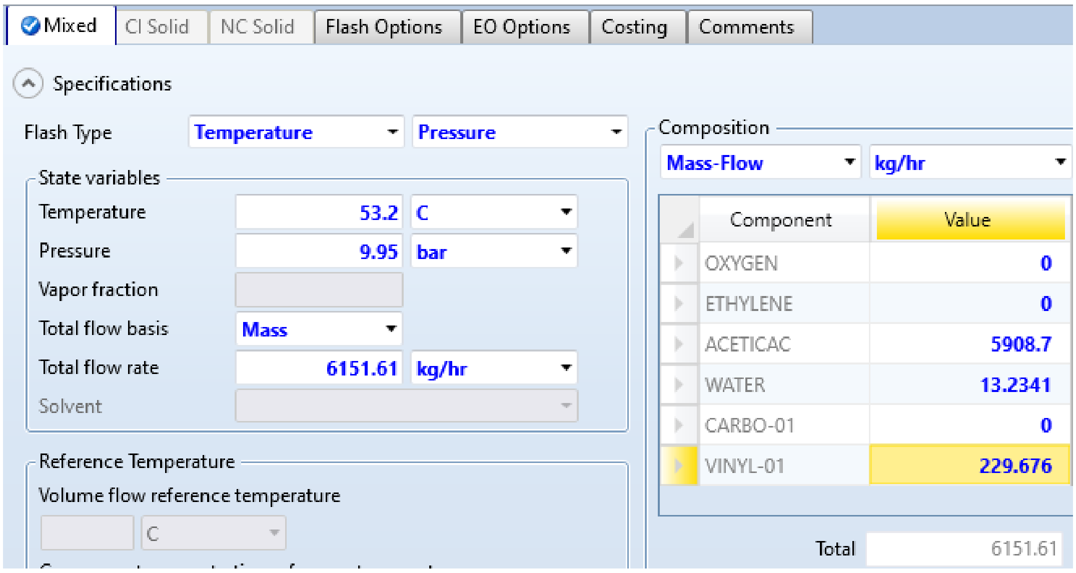
Reference Temperature

Volume flow reference temperature: C

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 2.2204 |
| ETHYLENE | 239.896 |
| ACETICAC | 5115.55 |
| WATER | 239.896 |
| CARBO-01 | 187.676 |
| VINYL-01 | 2280.3 |
| Total | 8065.54 |

### S19 Specifications:



Specifications

Flash Type: Temperature, Pressure

State variables

- Temperature: 53.2 C
- Pressure: 9.95 bar
- Vapor fraction:
- Total flow basis: Mass
- Total flow rate: 6151.61 kg/hr
- Solvent:

Reference Temperature

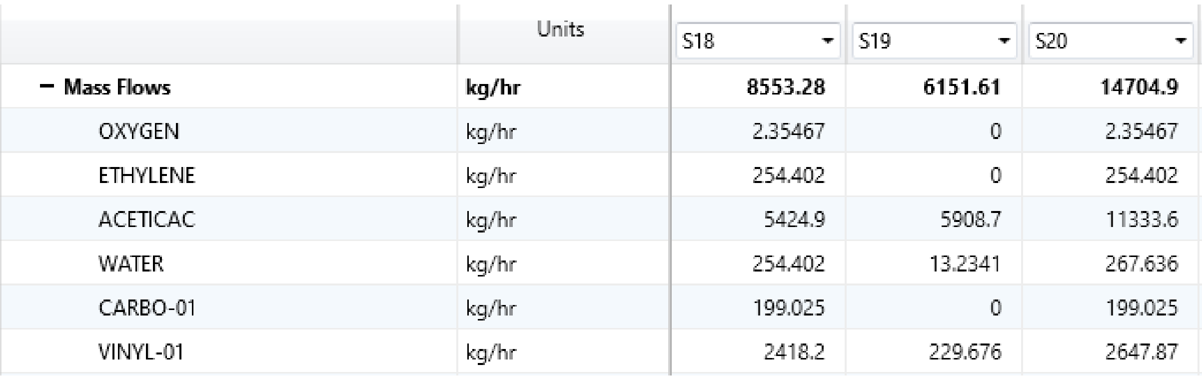
Volume flow reference temperature: C

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 0 |
| ETHYLENE | 0 |
| ACETICAC | 5908.7 |
| WATER | 13.2341 |
| CARBO-01 | 0 |
| VINYL-01 | 229.676 |

Total 6151.61

### Stream Results of Mixer:



| | Units | S18 | S19 | S20 |
|---|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **8553.28** | **6151.61** | **14704.9** |
| OXYGEN | kg/hr | 2.35467 | 0 | 2.35467 |
| ETHYLENE | kg/hr | 254.402 | 0 | 254.402 |
| ACETICAC | kg/hr | 5424.9 | 5908.7 | 11333.6 |
| WATER | kg/hr | 254.402 | 13.2341 | 267.636 |
| CARBO-01 | kg/hr | 199.025 | 0 | 199.025 |
| VINYL-01 | kg/hr | 2418.2 | 229.676 | 2647.87 |

### 11.2.5. Heat Exchanger:

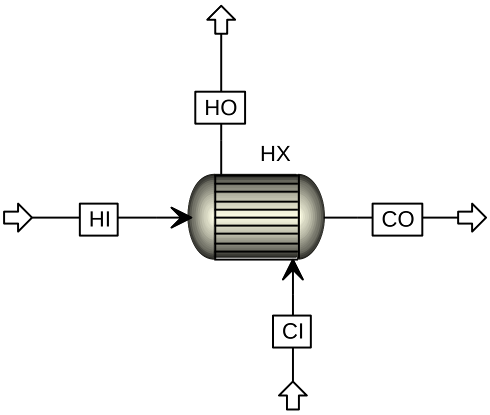
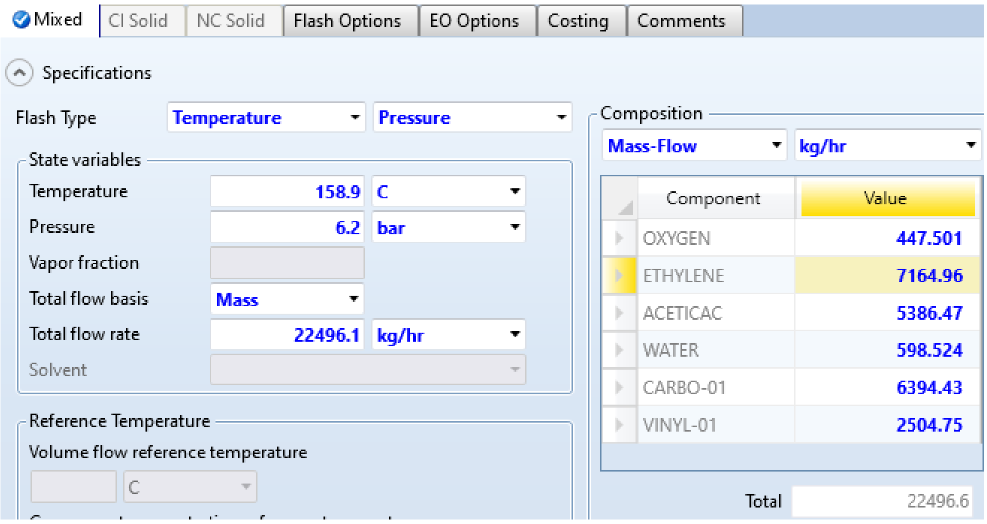


**Figure 21:** Simulated figure of Heat Exchanger

## Hot Stream Specifications:



Flash Type: Temperature, Pressure

State variables

| | | |
|---|---|---|
| Temperature | 158.9 | C |
| Pressure | 6.2 | bar |
| Vapor fraction | | |
| Total flow basis | Mass | |
| Total flow rate | 22496.1 | kg/hr |
| Solvent | | |

Reference Temperature

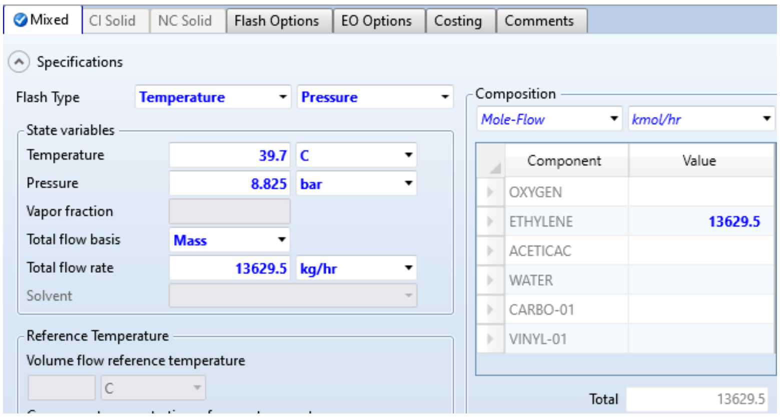
Volume flow reference temperature: C

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 447.501 |
| ETHYLENE | 7164.96 |
| ACETICAC | 5386.47 |
| WATER | 598.524 |
| CARBO-01 | 6394.43 |
| VINYL-01 | 2504.75 |

Total: 22496.6

## Cold Stream Specifications:



Flash Type: Temperature, Pressure

State variables

| | | |
|---|---|---|
| Temperature | 39.7 | C |
| Pressure | 8.825 | bar |
| Vapor fraction | | |
| Total flow basis | Mass | |
| Total flow rate | 13629.5 | kg/hr |
| Solvent | | |

Reference Temperature

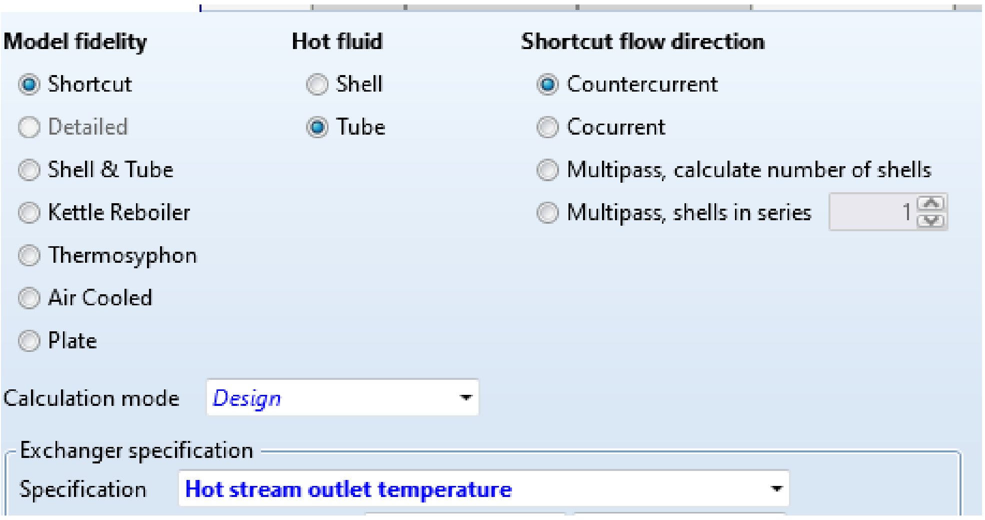
Volume flow reference temperature: C

Composition: Mole-Flow, kmol/hr

| Component | Value |
|---|---|
| OXYGEN | |
| ETHYLENE | 13629.5 |
| ACETICAC | |
| WATER | |
| CARBO-01 | |
| VINYL-01 | |

Total: 13629.5

## Heat Exchanger Specifications:



**Model fidelity**
- ● Shortcut
- ○ Detailed
- ○ Shell & Tube
- ○ Kettle Reboiler
- ○ Thermosyphon
- ○ Air Cooled
- ○ Plate

**Hot fluid**
- ○ Shell
- ● Tube

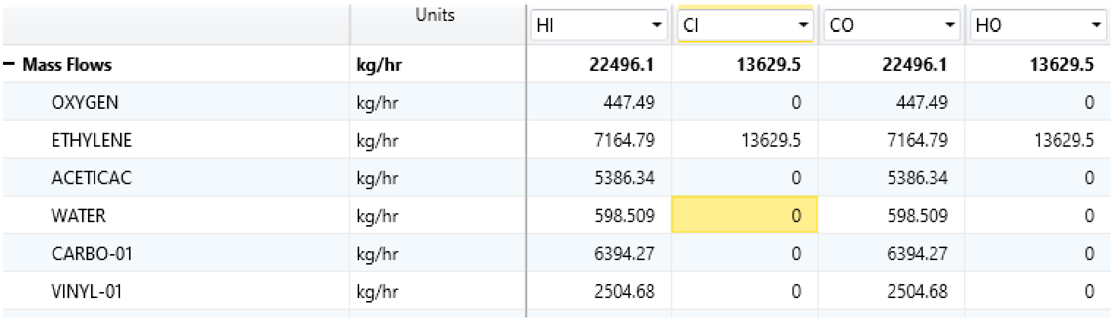
**Shortcut flow direction**
- ● Countercurrent
- ○ Cocurrent
- ○ Multipass, calculate number of shells
- ○ Multipass, shells in series 1

Calculation mode: Design

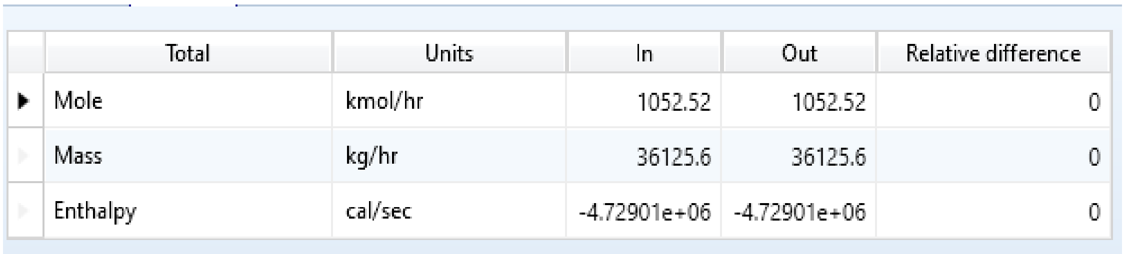
Exchanger specification

Specification: Hot stream outlet temperature

## Stream Results of Mixer:

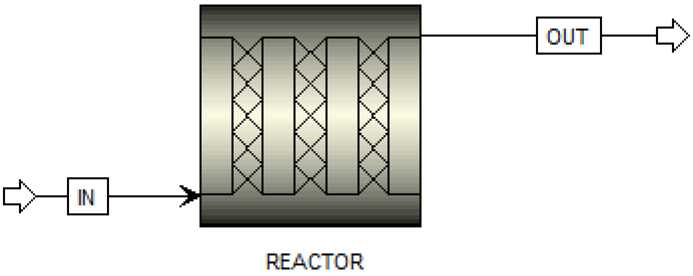


| | Units | HI | CI | CO | HO |
|---|---|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **22496.1** | **13629.5** | **22496.1** | **13629.5** |
| OXYGEN | kg/hr | 447.49 | 0 | 447.49 | 0 |
| ETHYLENE | kg/hr | 7164.79 | 13629.5 | 7164.79 | 13629.5 |
| ACETICAC | kg/hr | 5386.34 | 0 | 5386.34 | 0 |
| WATER | kg/hr | 598.509 | 0 | 598.509 | 0 |
| CARBO-01 | kg/hr | 6394.27 | 0 | 6394.27 | 0 |
| VINYL-01 | kg/hr | 2504.68 | 0 | 2504.68 | 0 |

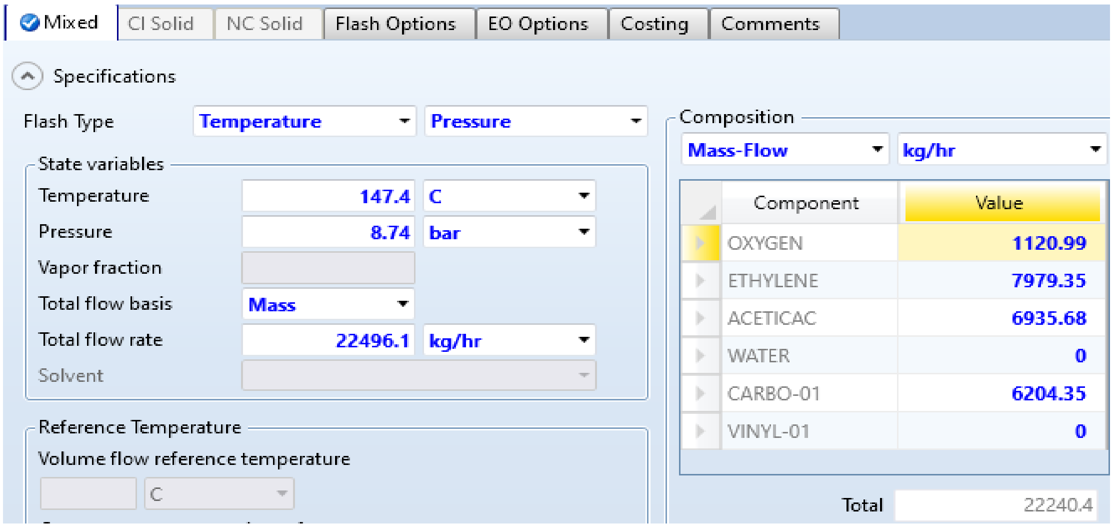


| Total | Units | In | Out | Relative difference |
|---|---|---|---|---|
| Mole | kmol/hr | 1052.52 | 1052.52 | 0 |
| Mass | kg/hr | 36125.6 | 36125.6 | 0 |
| Enthalpy | cal/sec | -4.72901e+06 | -4.72901e+06 | 0 |

### 11.2.6. Reactor:



## Feed Specification:



Flash Type: Temperature, Pressure

State variables

Temperature: 147.4 C

Pressure: 8.74 bar

Vapor fraction:

Total flow basis: Mass

Total flow rate: 22496.1 kg/hr

Solvent:

Reference Temperature

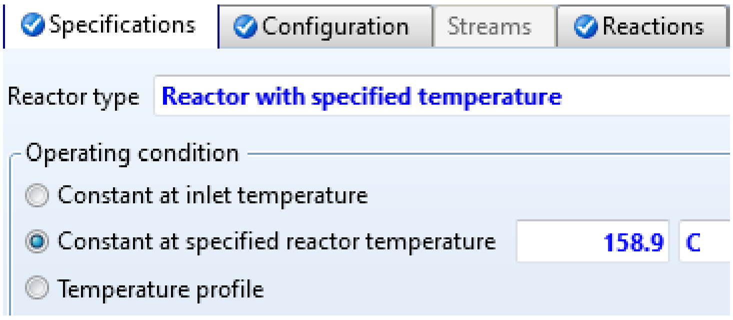
Volume flow reference temperature: C

Composition: Mass-Flow, kg/hr

| Component | Value |
|---|---|
| OXYGEN | 1120.99 |
| ETHYLENE | 7979.35 |
| ACETICAC | 6935.68 |
| WATER | 0 |
| CARBO-01 | 6204.35 |
| VINYL-01 | 0 |

Total: 22240.4

## Reactor Specification:



Reactor type: Reactor with specified temperature

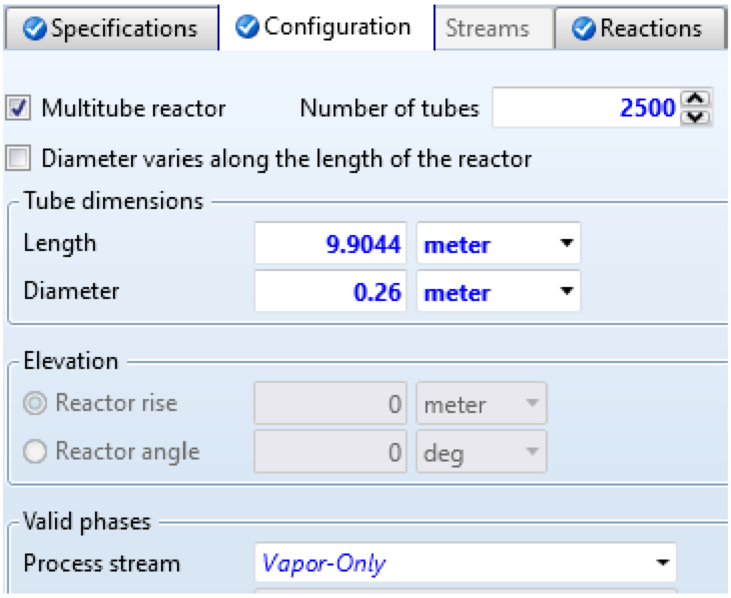
Operating condition

○ Constant at inlet temperature

● Constant at specified reactor temperature 158.9 C

○ Temperature profile

## Reactor Configuration:



☑ Multitube reactor Number of tubes 2500

☐ Diameter varies along the length of the reactor

Tube dimensions

Length 9.9044 meter

Diameter 0.26 meter

Elevation

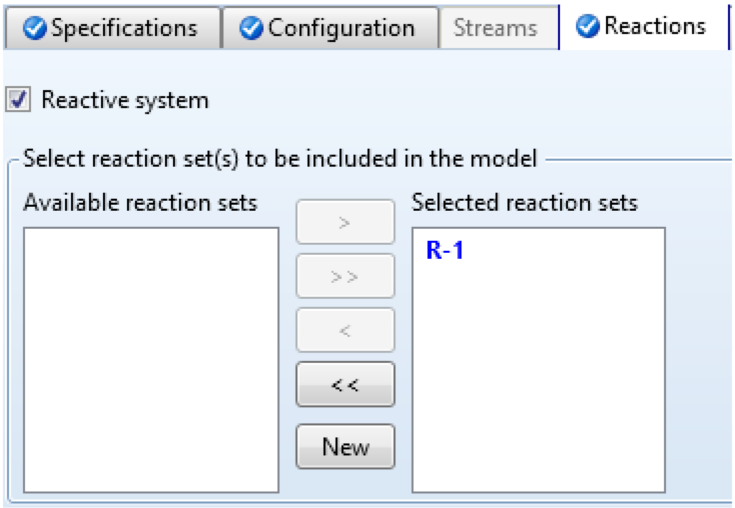
○ Reactor rise 0 meter

○ Reactor angle 0 deg

Valid phases

Process stream Vapor-Only

## Reactions:



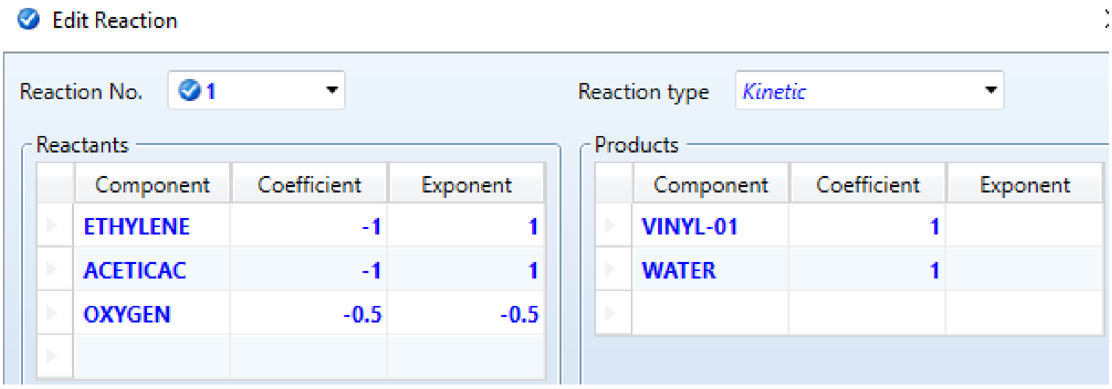
☑ Reactive system

Select reaction set(s) to be included in the model

Available reaction sets

Selected reaction sets: R-1

**Coefficient and Exponent:**



Reaction No. 1

Reaction type Kinetic

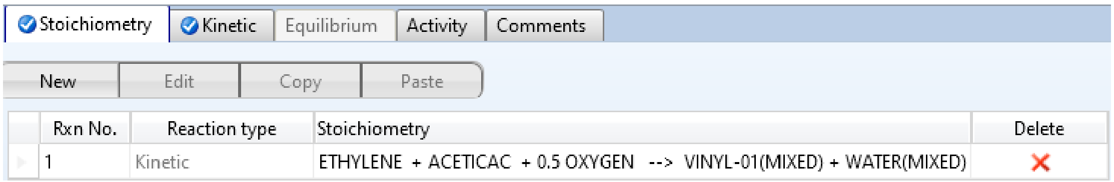
Reactants

| Component | Coefficient | Exponent |
|---|---|---|
| ETHYLENE | -1 | 1 |
| ACETICAC | -1 | 1 |
| OXYGEN | -0.5 | -0.5 |
| | | |

Products

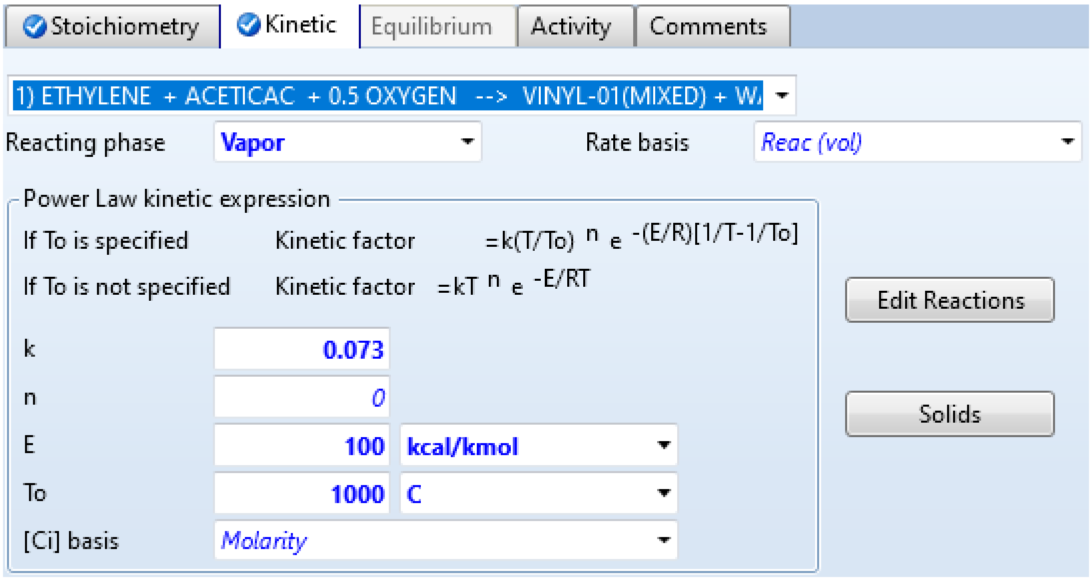
| Component | Coefficient | Exponent |
|---|---|---|
| VINYL-01 | 1 | |
| WATER | 1 | |
| | | |

**Stoichiometry of Reactor:**



| Rxn No. | Reaction type | Stoichiometry | Delete |
|---|---|---|---|
| 1 | Kinetic | ETHYLENE + ACETICAC + 0.5 OXYGEN --> VINYL-01(MIXED) + WATER(MIXED) | ✕ |

**Kinetic of Reactor:**



1) ETHYLENE + ACETICAC + 0.5 OXYGEN --> VINYL-01(MIXED) + W

Reacting phase Vapor

Rate basis Reac (vol)

Power Law kinetic expression

If To is specified Kinetic factor $=k(T/To)^{n}\ e^{-(E/R)[1/T-1/To]}$

If To is not specified Kinetic factor $=kT^{n}\ e^{-E/RT}$

k 0.073

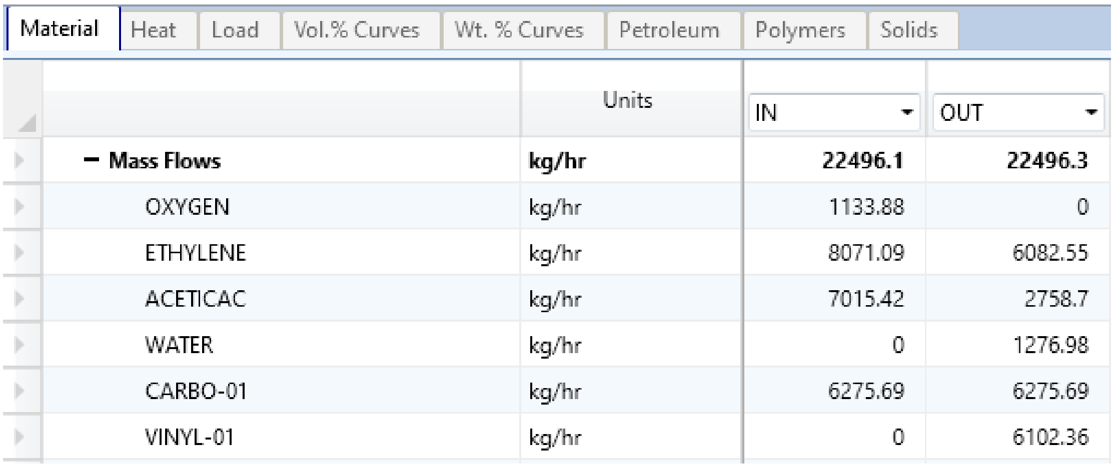
n 0

E 100 kcal/kmol

To 1000 C

[Ci] basis Molarity

## Stream Results:



|  | Units | IN | OUT |
|---|---|---|---|
| **− Mass Flows** | **kg/hr** | **22496.1** | **22496.3** |
| OXYGEN | kg/hr | 1133.88 | 0 |
| ETHYLENE | kg/hr | 8071.09 | 6082.55 |
| ACETICAC | kg/hr | 7015.42 | 2758.7 |
| WATER | kg/hr | 0 | 1276.98 |
| CARBO-01 | kg/hr | 6275.69 | 6275.69 |
| VINYL-01 | kg/hr | 0 | 6102.36 |

# Chapter 12

# Layout

The lucrative erection and performance of a process unit based on how good the plant equipment are defined on the process flow sheet. The primary elements to be appraised are following that must be in mind in designing plant layout are as follows:

- Economic compensation; erection and operation cost
- The process prerequisites
- Ease of operation
- Ease of maintenance
- Safety
- Future expansion

## 12.1.Economic Compensation:

The price of erection could be decreased by selecting an arrangement that provides the smallest path of joining pipes across instruments and by selecting minimum price of steel art. That would not be the primarily ideal joining for functioning and preservation.

## 12.2.Process Pre-requisite:

The necessary equipment must be installed ideally in the process. Even the fitting of the small accessories should be in such manner that they will cover the minimum space.

## 12.3.Ease of operation:

Equipment which are necessary for operation must be present at suitable position. Necessary valves and instruments should also be at ease position and height. Enough place for work should be provide so that the excess on equipment is easy.

## 12.4.Ease of Maintenance:

For maintenance all the equipment sited properly for example distillation columns have re-boilers and condensers which can be replaced in case of any failure. Similarly, other equipment’s which are needed to be maintained such as heat exchangers and pumps, compressors should be present at ease position.

## 12.5.Safety:

Protective restrictions should be designed necessarily for separating the risky appliances for lessen the effect any discharge. Minimum three emergency exists should be installed to the explosive process site. Highly hazardous storage must be well protective.

## 12.6.Future Expansion:

Equipment should be located so that it can be conveniently tied in with any future expansion of the process. Space should be left for the pipes for future needs, and service pipes over-sized to allow for future requirements to control and for safety issues.

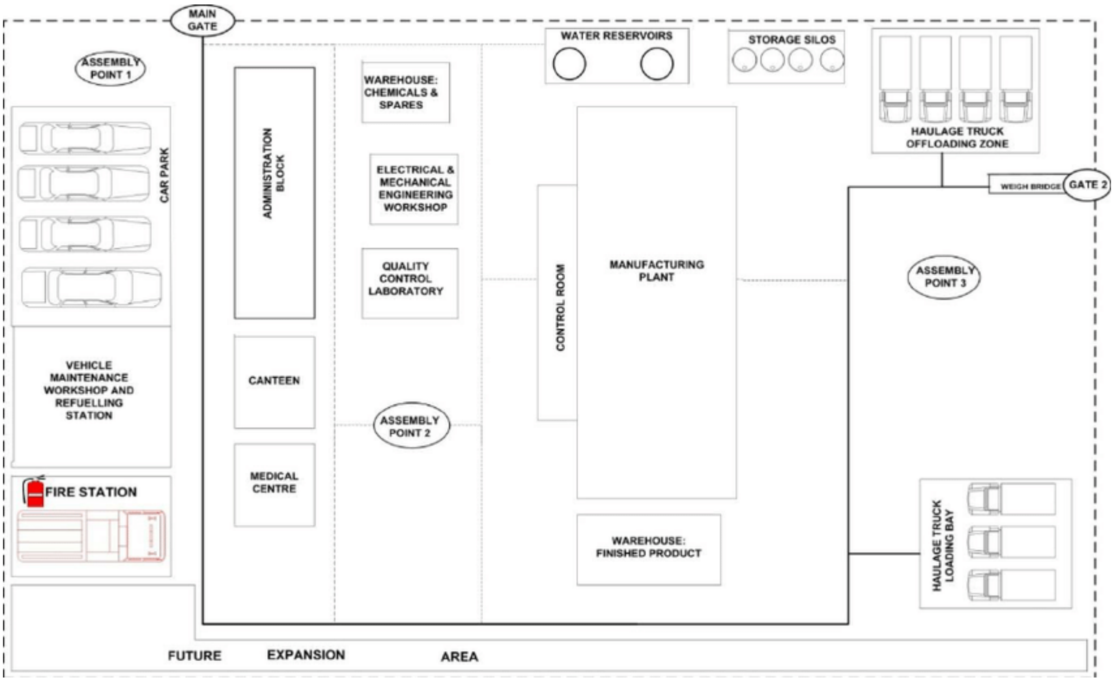


**Figure 22:** Layout display of VAM plant

# Chapter 13

# Sustainability Development Goals

The United Nation 17 Sustainability development goals are given as:

1. End poverty in all its form. ☑
2. Eradicate famine and hunger. ☐
3. Guarantee healthy lives and promote well-being for all. ☐
4. Ensure education and learning opportunities for all. ☐
5. Ensure that women and girls have the same rights and opportunities as men. ☐
6. Provide availability of water and sanitation. ☐
7. Ensure access to affordable, reliable, sustainable and modern energy for all ☐
8. Promote sustained, inclusive and sustainable economic growth, full and productive employment and decent work for all ☑
9. Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation ☑
10. Reduce inequality within and among countries ☐
11. Make cities and human settlements inclusive, safe, resilient and sustainable ☐
12. Ensure sustainable consumption and production patterns ☑
13. Take urgent action to combat climate change and its impacts ☐
14. Conserve and sustainably use the oceans, seas and marine resources ☐
15. Protect, restore and promote sustainable use of terrestrial ecosystems ☐
16. Promote peaceful and inclusive societies for sustainable development ☐
17. Strengthen the means of implementation and revitalize the global partnership ☑

The Sustainable Development Goals (SDGs) are a set of laws and regulations that attempt to achieve various development objectives for the benefit of the planet and its inhabitants. Industries have a great deal of potential to support a variety of SDGs through their core business operations by offering products and services that support the SDGs both domestically and internationally. Some of the few SDGs that will be met by our initiative:

**Table 50:** Sustainability development goals

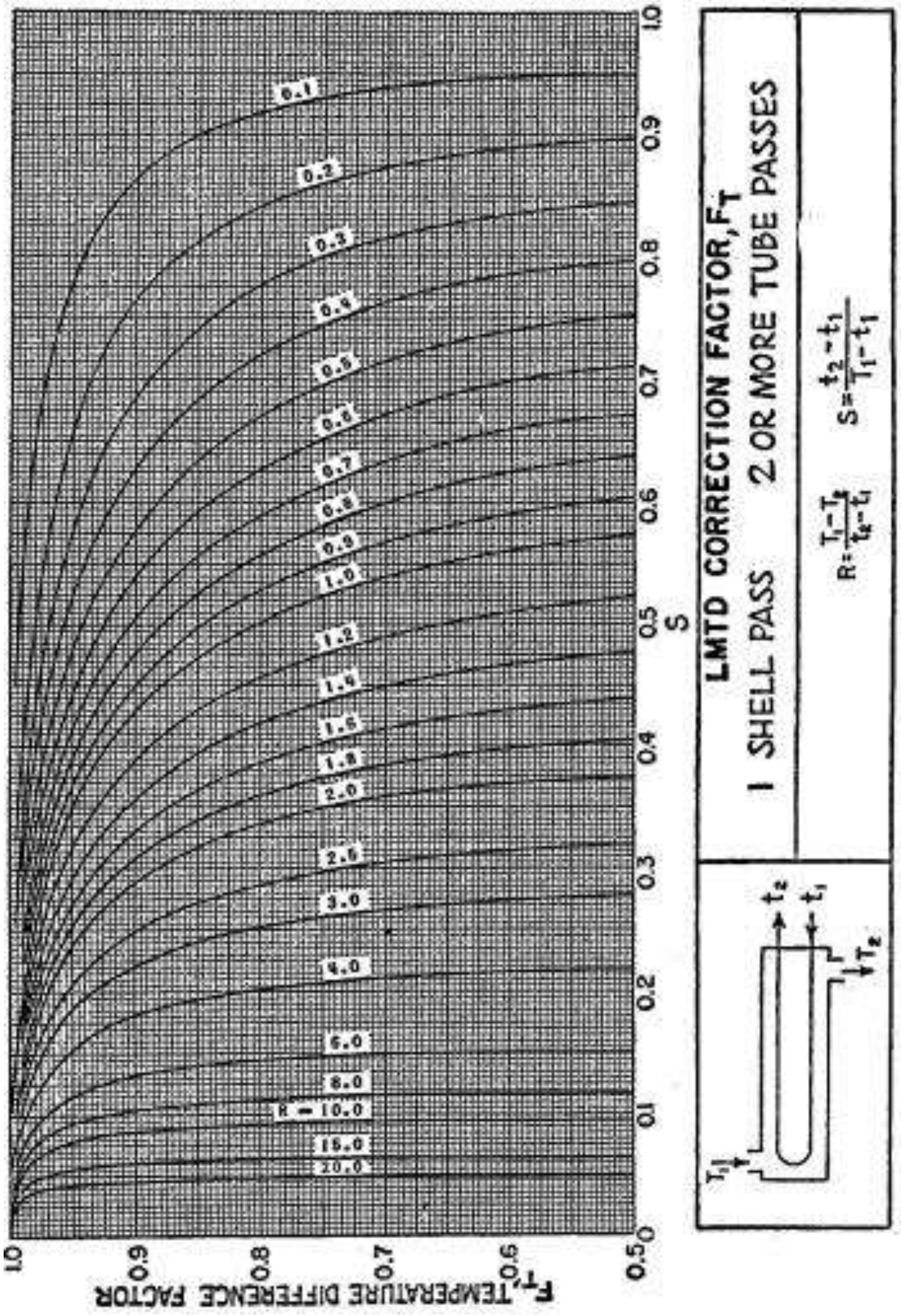
| Sr.No | Goal | SDGs | Related to our project |
|---|---|---|---|
| **1** | **Goal 1:**<br>No Poverty. | The objective is to remove poverty | Unemployment and poverty is reduced by installation of these types of chemical Plants. Chemical process industries play a critical role in Job creation. |
| **2** | **Goal 8:**<br>Decent work and economic growth | The objective is to create favorable conditions that promote the availability of quality jobs, which in turn stimulate economic growth. | Our project will follow this goal as an entrepreneurial opportunity creates more job opportunities for society, and economic growth will be improved by ensuring:<br>- Youth employment and training of low-wage employees will boost economic growth.<br>- Improving workforce training will boost the plant's overall output.<br>- Moreover, higher grade machinery will be used to increase production. |
| **3** | **Goal 9**:<br>Industry innovation and infrastructure. | This objective is to encourage fair and sustainable industrial growth, with a focus on increasing employment opportunities and contributing to the overall economic growth of a country. It includes | This objective is critical to the project since exporting VAM will attempt to enhance the country's economy and grow GDP.<br>- Productivity can be increased by creating a strong and resilient infrastructure of the |

| | | | |
|---|---|---|---|
| | | specific targets such as doubling the industrial sector's share of employment and GDP, particularly in underdeveloped nations. | industry, it will promote economic growth and improve access to enterprises<br>- Moreover, improvement in infrastructure and enhancement in research could be implemented for better sustainability and economic growth. |
| **4** | **Goal 12:** Responsible consumption and production. | Sustainable consumption and production aim to achieve better and more efficient use of resources while reducing environmental impacts. It involves the use of environmentally friendly products and services and promoting lifestyles that are sustainable and less wasteful. | Sustainable consumption and production are a main goal that the project relates to. Responsible consumption of energy and raw material will implement this goal. Heat & energy integration research of the entire plant will decrease the cost needed for energy and improve the resource efficiency. The cost saved can be utilized in further research. Separation and purification of the raw material (in our case, oxy acetylation) will further improve resource efficiency and sustainability. |
| **5** | **Goal 17:** Partnerships for the goals. | In order to achieve sustainable development, the declaration emphasizes the necessity of enhancing implementation mechanisms and inter-national collaboration. It draws attention to the significance of global support and investments for the advancement of new technologies. | Partnerships with various firms in several countries help improve exports and trades of the product. Since VAM market will grow at 4-5% (CAGR), the demand of VAM will increase and by increasing partnerships, export of VAM will increase. Global trade of VAM will target the GDP of Pakistan and will promote economic growth. |

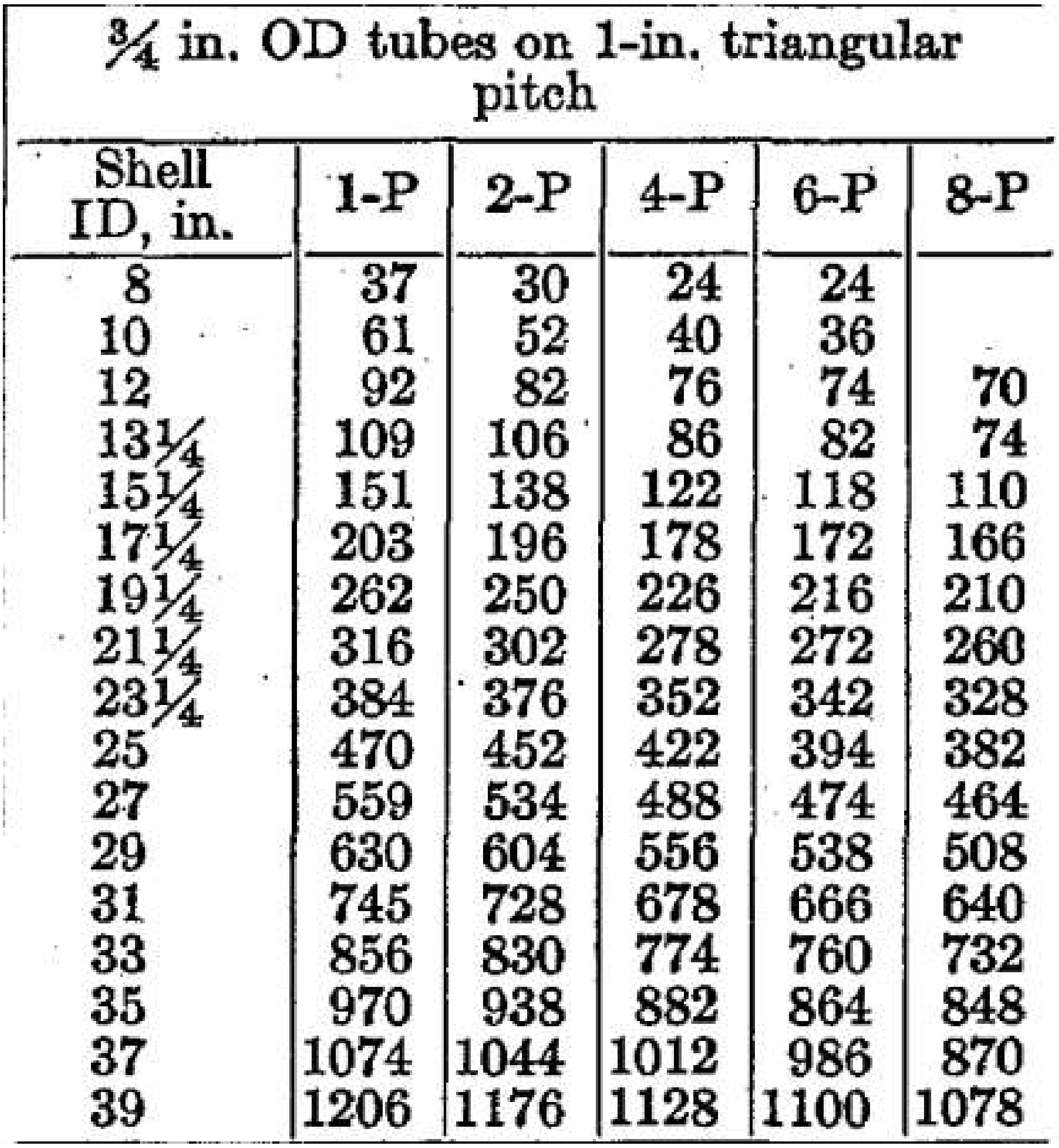
# Chapter 14

# Appendix

Appendix A: LMTD correction factors for 1-2 exchangers



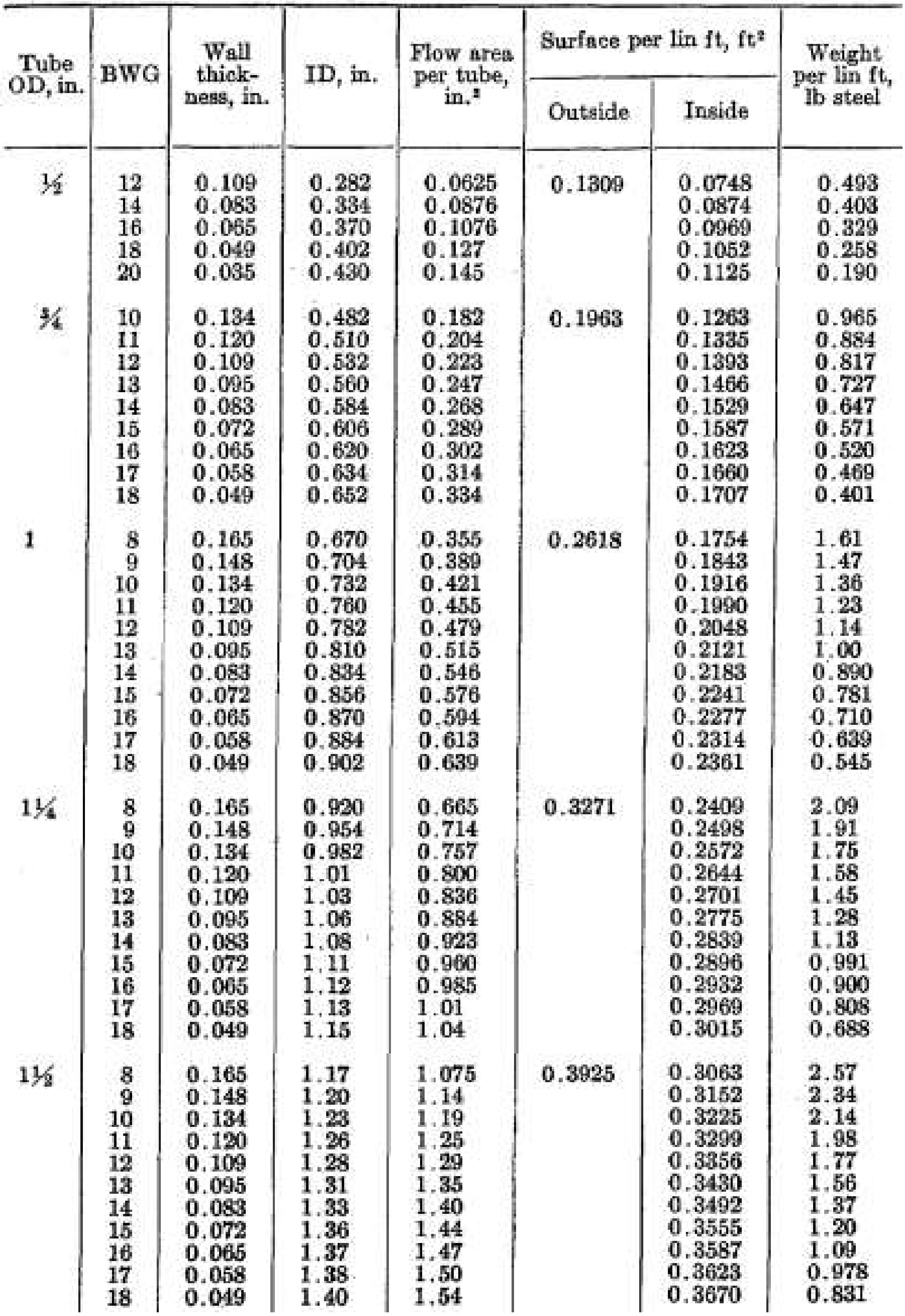
**Appendix B:** Tube sheet layouts Triangular Pitch



¾ in. OD tubes on 1-in. triangular pitch

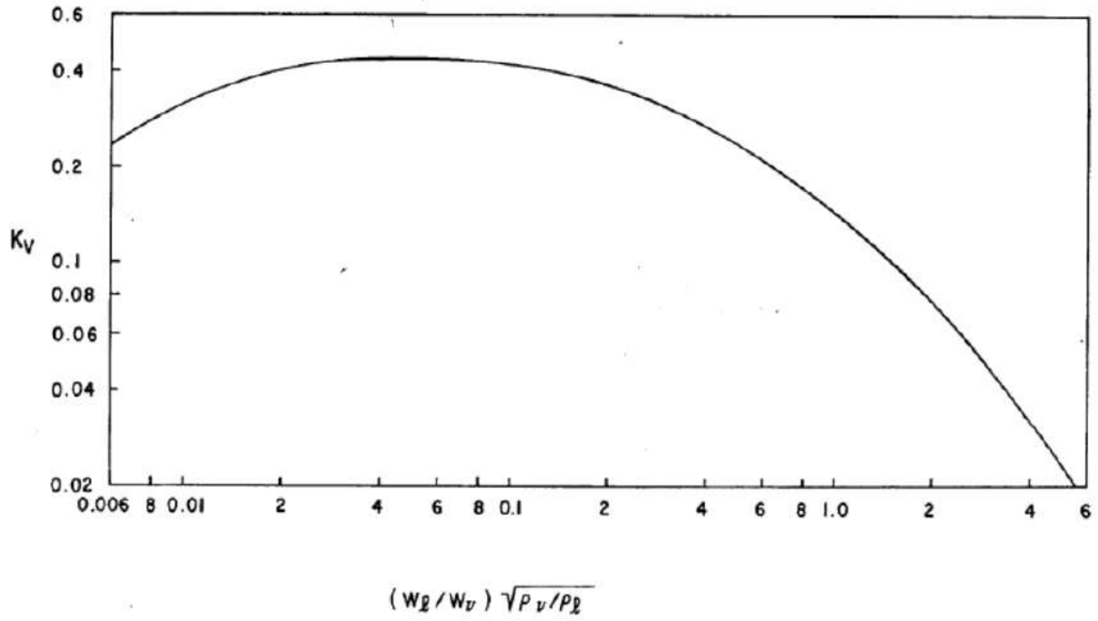
| Shell ID, in. | 1-P | 2-P | 4-P | 6-P | 8-P |
|---|---|---|---|---|---|
| 8 | 37 | 30 | 24 | 24 | |
| 10 | 61 | 52 | 40 | 36 | |
| 12 | 92 | 82 | 76 | 74 | 70 |
| 13¼ | 109 | 106 | 86 | 82 | 74 |
| 15¼ | 151 | 138 | 122 | 118 | 110 |
| 17¼ | 203 | 196 | 178 | 172 | 166 |
| 19¼ | 262 | 250 | 226 | 216 | 210 |
| 21¼ | 316 | 302 | 278 | 272 | 260 |
| 23¼ | 384 | 376 | 352 | 342 | 328 |
| 25 | 470 | 452 | 422 | 394 | 382 |
| 27 | 559 | 534 | 488 | 474 | 464 |
| 29 | 630 | 604 | 556 | 538 | 508 |
| 31 | 745 | 728 | 678 | 666 | 640 |
| 33 | 856 | 830 | 774 | 760 | 732 |
| 35 | 970 | 938 | 882 | 864 | 848 |
| 37 | 1074 | 1044 | 1012 | 986 | 870 |
| 39 | 1206 | 1176 | 1128 | 1100 | 1078 |

**Appendix C:** Heat Exchanger and Condenser tube data

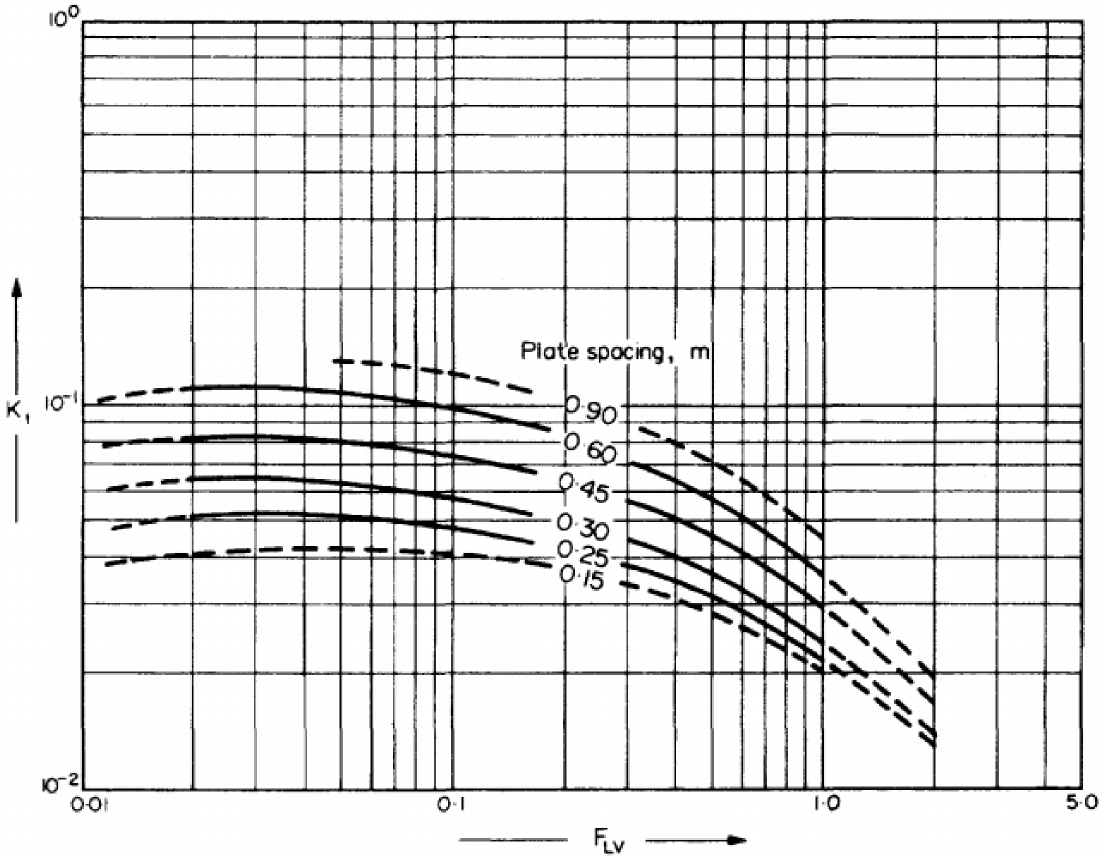


| Tube OD, in. | BWG | Wall thickness, in. | ID, in. | Flow area per tube, in.$^2$ | Surface per lin ft, ft$^2$ |  | Weight per lin ft, lb steel |
|---|---|---|---|---|---|---|---|
|  |  |  |  |  | Outside | Inside |  |
| ½ | 12 | 0.109 | 0.282 | 0.0625 | 0.1309 | 0.0748 | 0.493 |
|  | 14 | 0.083 | 0.334 | 0.0876 |  | 0.0874 | 0.403 |
|  | 16 | 0.065 | 0.370 | 0.1076 |  | 0.0969 | 0.329 |
|  | 18 | 0.049 | 0.402 | 0.127 |  | 0.1052 | 0.258 |
|  | 20 | 0.035 | 0.430 | 0.145 |  | 0.1125 | 0.190 |
| ¾ | 10 | 0.134 | 0.482 | 0.182 | 0.1963 | 0.1263 | 0.965 |
|  | 11 | 0.120 | 0.510 | 0.204 |  | 0.1335 | 0.884 |
|  | 12 | 0.109 | 0.532 | 0.223 |  | 0.1393 | 0.817 |
|  | 13 | 0.095 | 0.560 | 0.247 |  | 0.1466 | 0.727 |
|  | 14 | 0.083 | 0.584 | 0.268 |  | 0.1529 | 0.647 |
|  | 15 | 0.072 | 0.606 | 0.289 |  | 0.1587 | 0.571 |
|  | 16 | 0.065 | 0.620 | 0.302 |  | 0.1623 | 0.520 |
|  | 17 | 0.058 | 0.634 | 0.314 |  | 0.1660 | 0.469 |
|  | 18 | 0.049 | 0.652 | 0.334 |  | 0.1707 | 0.401 |
| 1 | 8 | 0.165 | 0.670 | 0.355 | 0.2618 | 0.1754 | 1.61 |
|  | 9 | 0.148 | 0.704 | 0.389 |  | 0.1843 | 1.47 |
|  | 10 | 0.134 | 0.732 | 0.421 |  | 0.1916 | 1.36 |
|  | 11 | 0.120 | 0.760 | 0.455 |  | 0.1990 | 1.23 |
|  | 12 | 0.109 | 0.782 | 0.479 |  | 0.2048 | 1.14 |
|  | 13 | 0.095 | 0.810 | 0.515 |  | 0.2121 | 1.00 |
|  | 14 | 0.083 | 0.834 | 0.546 |  | 0.2183 | 0.890 |
|  | 15 | 0.072 | 0.856 | 0.576 |  | 0.2241 | 0.781 |
|  | 16 | 0.065 | 0.870 | 0.594 |  | 0.2277 | 0.710 |
|  | 17 | 0.058 | 0.884 | 0.613 |  | 0.2314 | 0.639 |
|  | 18 | 0.049 | 0.902 | 0.639 |  | 0.2361 | 0.545 |
| 1¼ | 8 | 0.165 | 0.920 | 0.665 | 0.3271 | 0.2409 | 2.09 |
|  | 9 | 0.148 | 0.954 | 0.714 |  | 0.2498 | 1.91 |
|  | 10 | 0.134 | 0.982 | 0.757 |  | 0.2572 | 1.75 |
|  | 11 | 0.120 | 1.01 | 0.800 |  | 0.2644 | 1.58 |
|  | 12 | 0.109 | 1.03 | 0.836 |  | 0.2701 | 1.45 |
|  | 13 | 0.095 | 1.06 | 0.884 |  | 0.2775 | 1.28 |
|  | 14 | 0.083 | 1.08 | 0.923 |  | 0.2839 | 1.13 |
|  | 15 | 0.072 | 1.11 | 0.960 |  | 0.2896 | 0.991 |
|  | 16 | 0.065 | 1.12 | 0.985 |  | 0.2932 | 0.900 |
|  | 17 | 0.058 | 1.13 | 1.01 |  | 0.2969 | 0.808 |
|  | 18 | 0.049 | 1.15 | 1.04 |  | 0.3015 | 0.688 |
| 1½ | 8 | 0.165 | 1.17 | 1.075 | 0.3925 | 0.3063 | 2.57 |
|  | 9 | 0.148 | 1.20 | 1.14 |  | 0.3152 | 2.34 |
|  | 10 | 0.134 | 1.23 | 1.19 |  | 0.3225 | 2.14 |
|  | 11 | 0.120 | 1.26 | 1.25 |  | 0.3299 | 1.98 |
|  | 12 | 0.109 | 1.28 | 1.29 |  | 0.3356 | 1.77 |
|  | 13 | 0.095 | 1.31 | 1.35 |  | 0.3430 | 1.56 |
|  | 14 | 0.083 | 1.33 | 1.40 |  | 0.3492 | 1.37 |
|  | 15 | 0.072 | 1.36 | 1.44 |  | 0.3555 | 1.20 |
|  | 16 | 0.065 | 1.37 | 1.47 |  | 0.3587 | 1.09 |
|  | 17 | 0.058 | 1.38 | 1.50 |  | 0.3623 | 0.978 |
|  | 18 | 0.049 | 1.40 | 1.54 |  | 0.3670 | 0.831 |

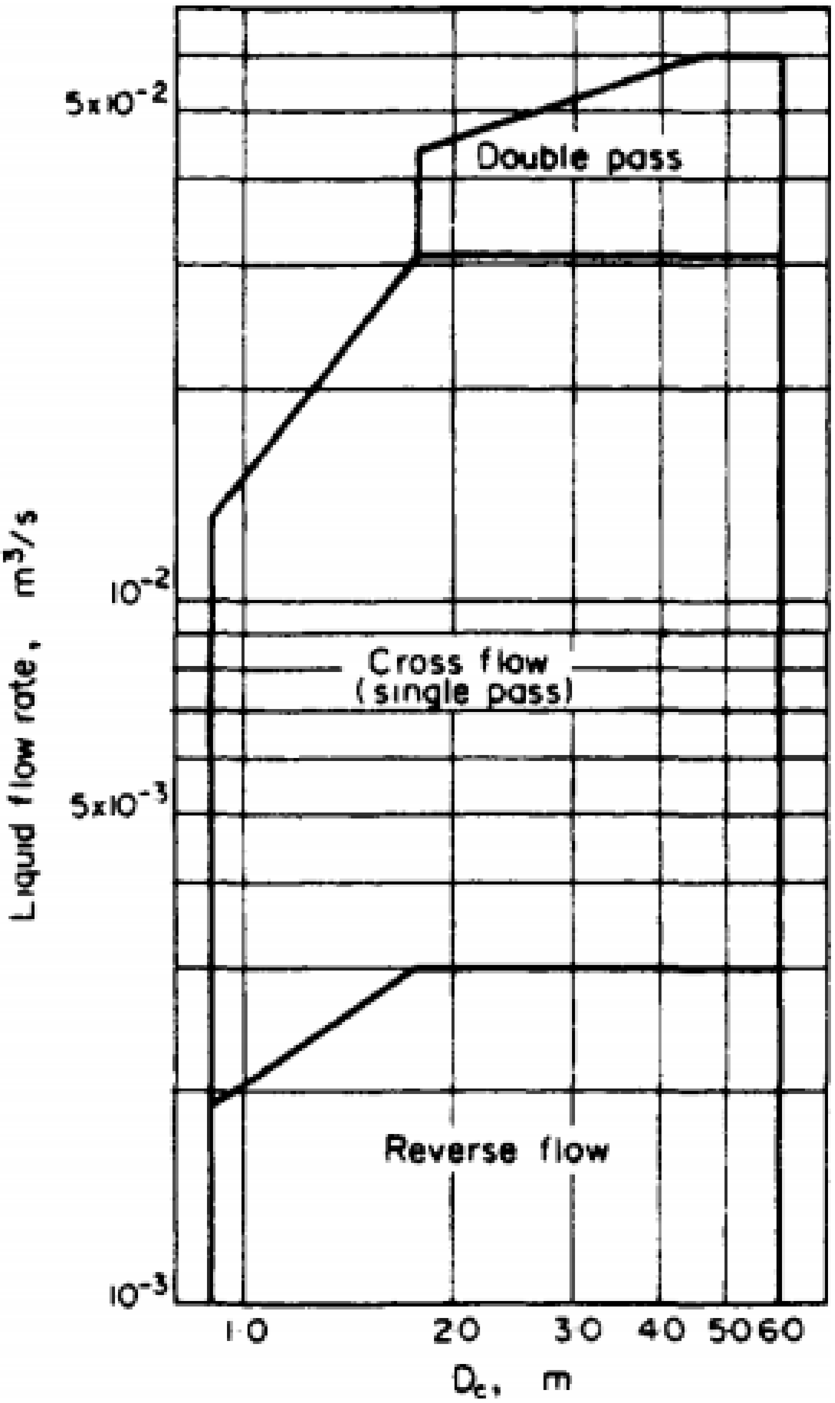
**ppendix D:** Design vapour velocity factor for vertical separators



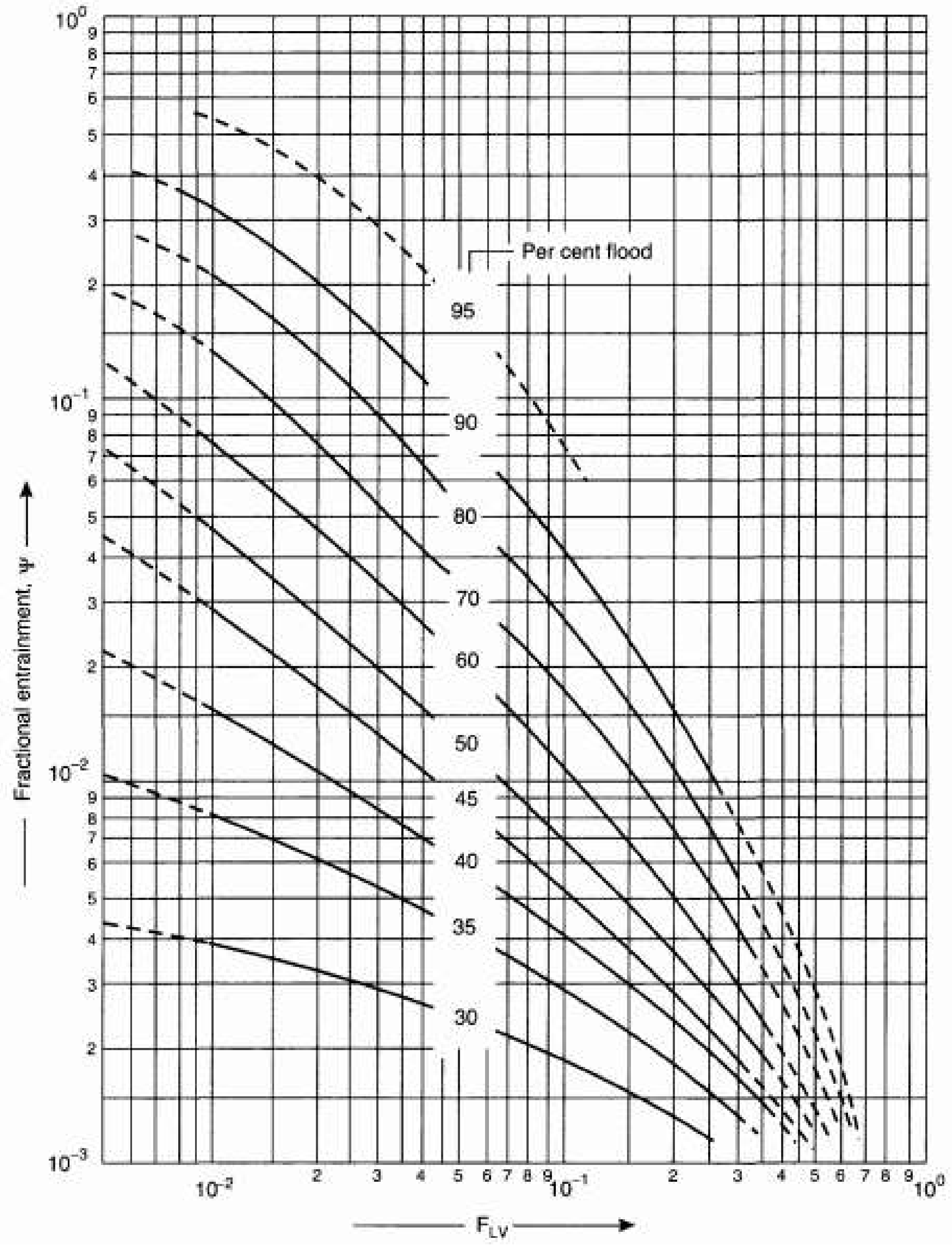
**Appendix E:** Flooding velocity, sieve plates



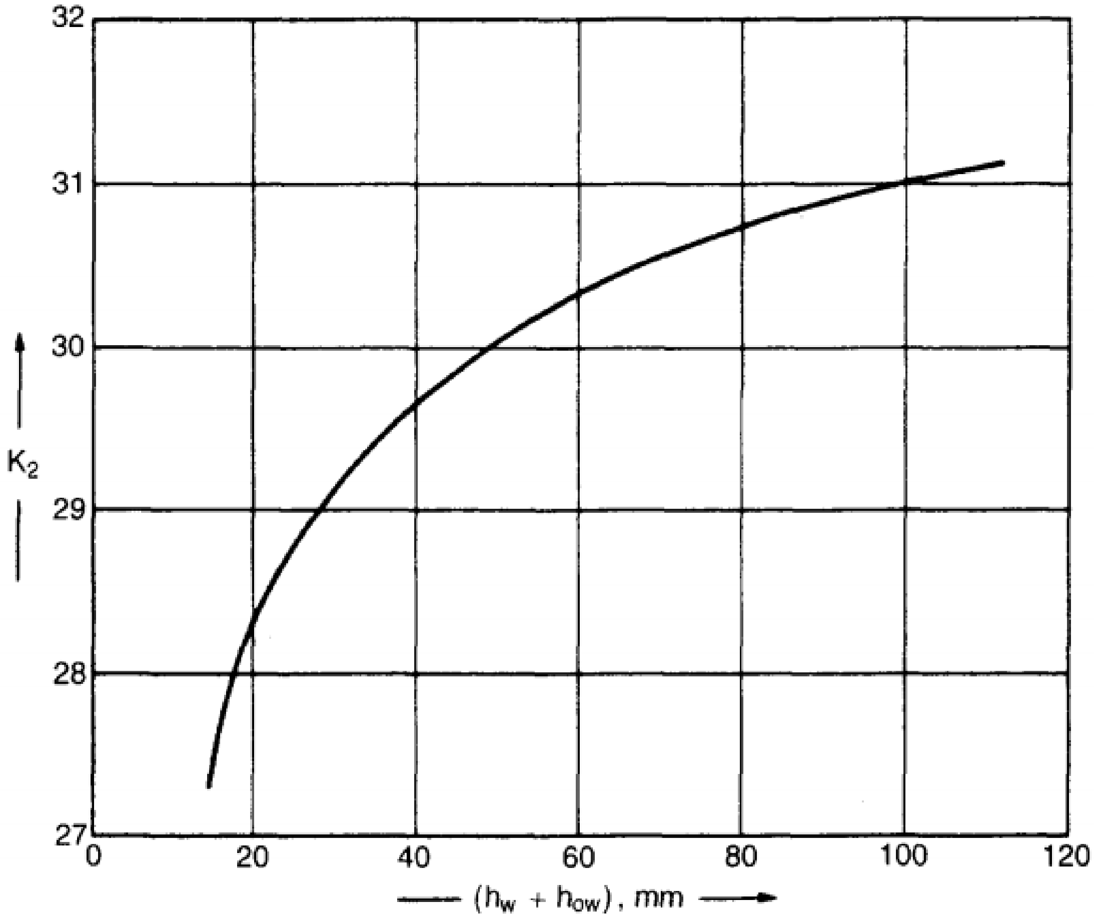
**Appendix F:** Selection of liquid-flow arrangement



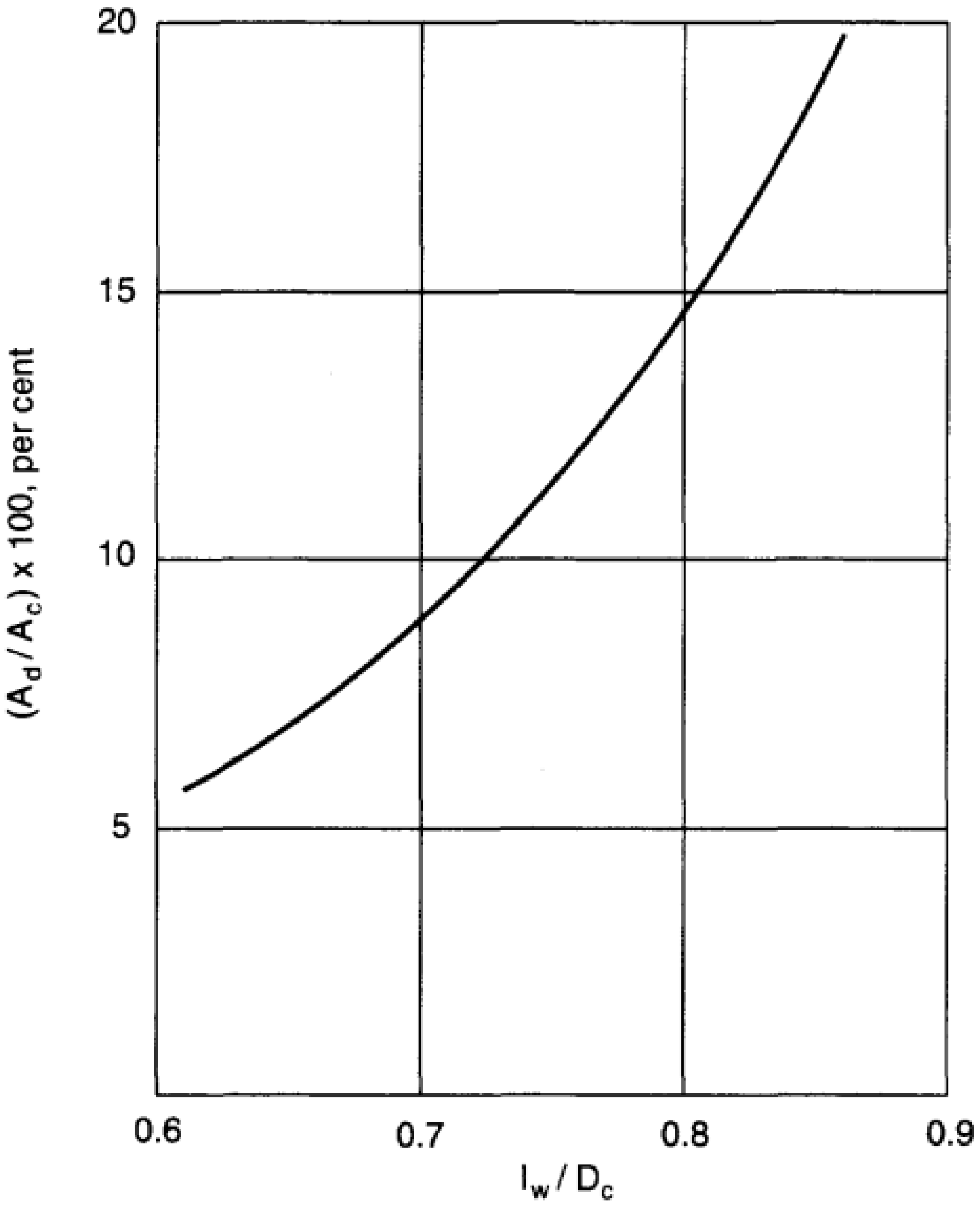
**Appendix G:** Entrainment correlation for sieve plates



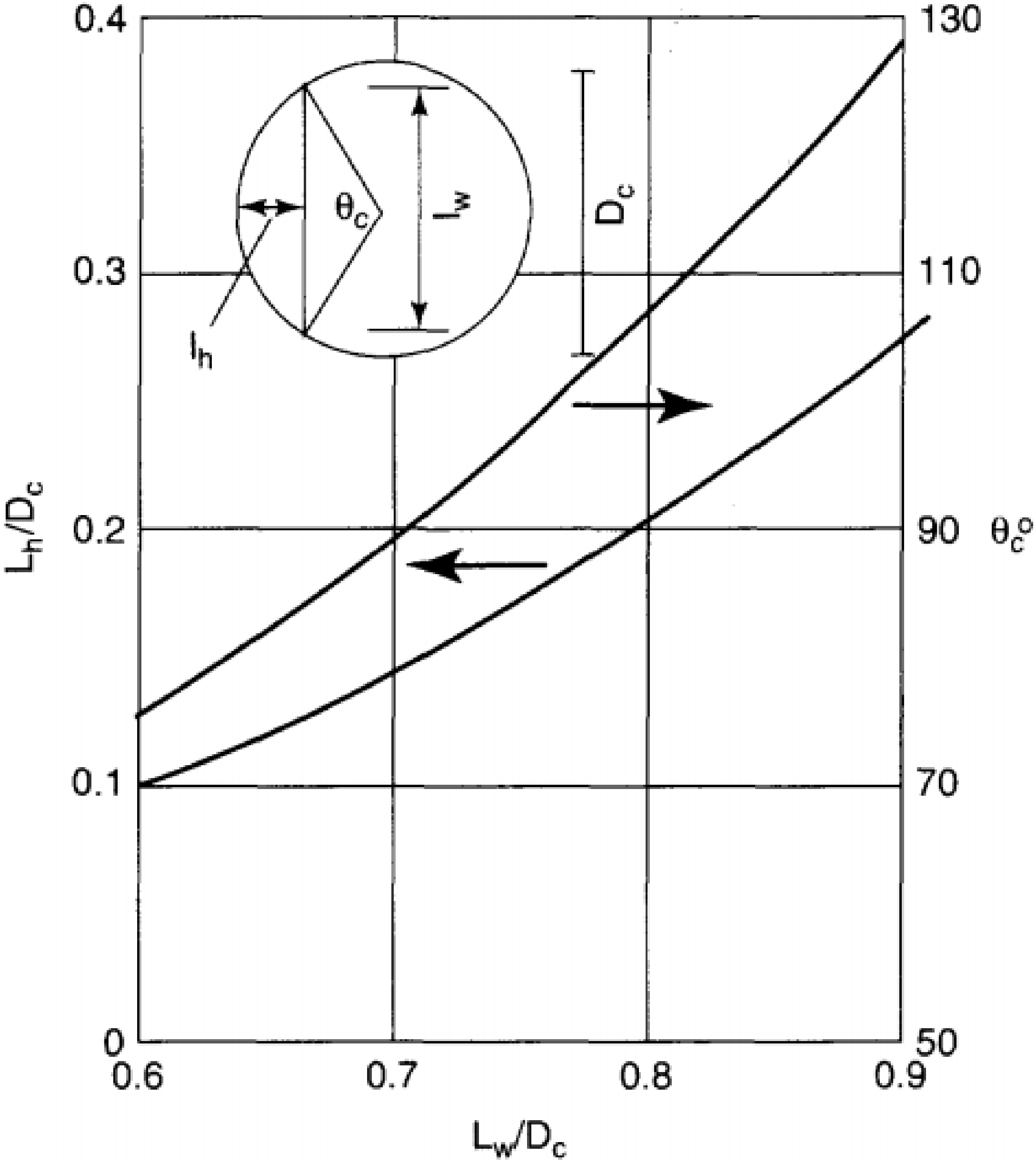
**Appendix H:** Weep-point correlation



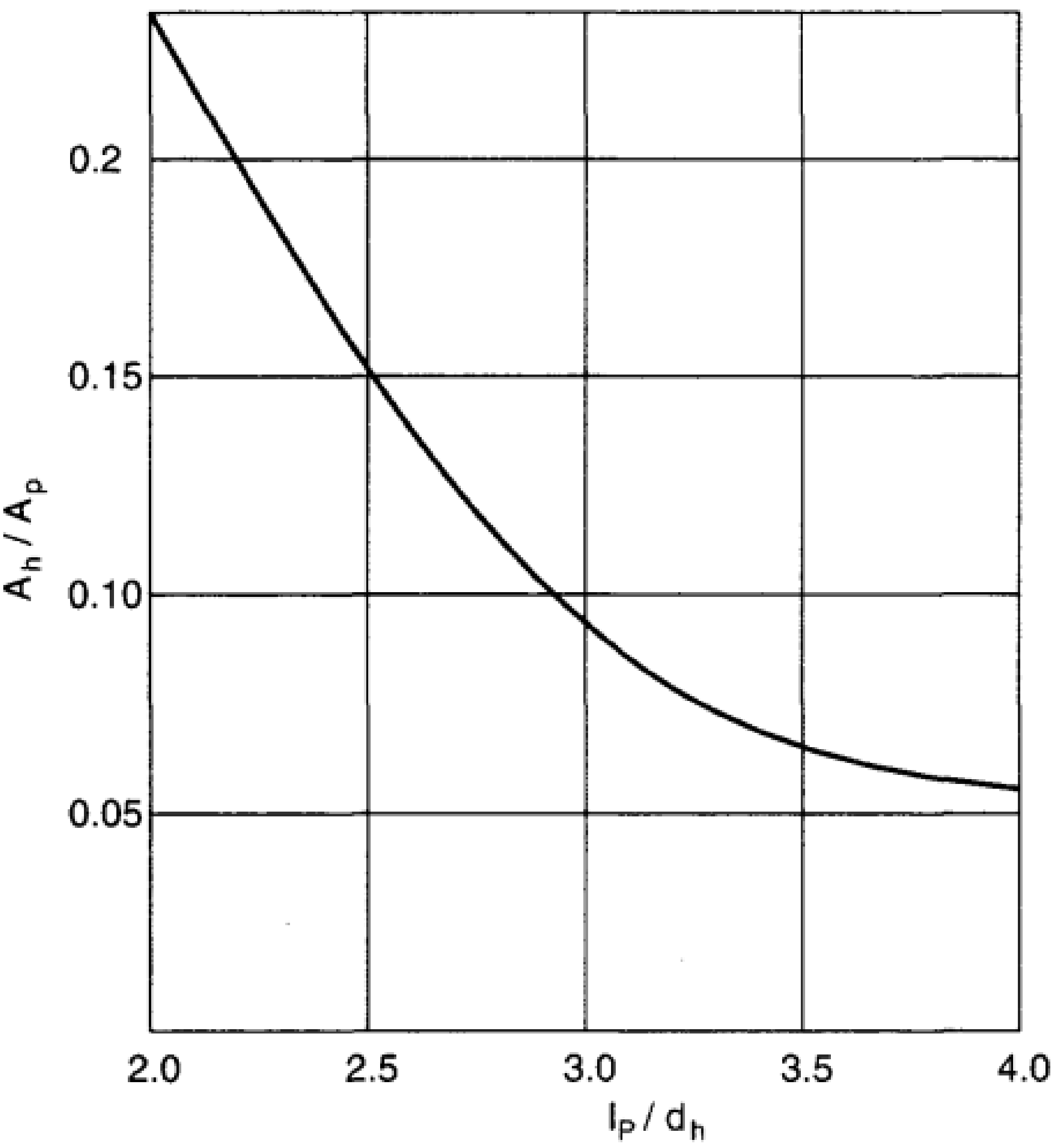
**Appendix I:** Relation between downcomer area and weir length



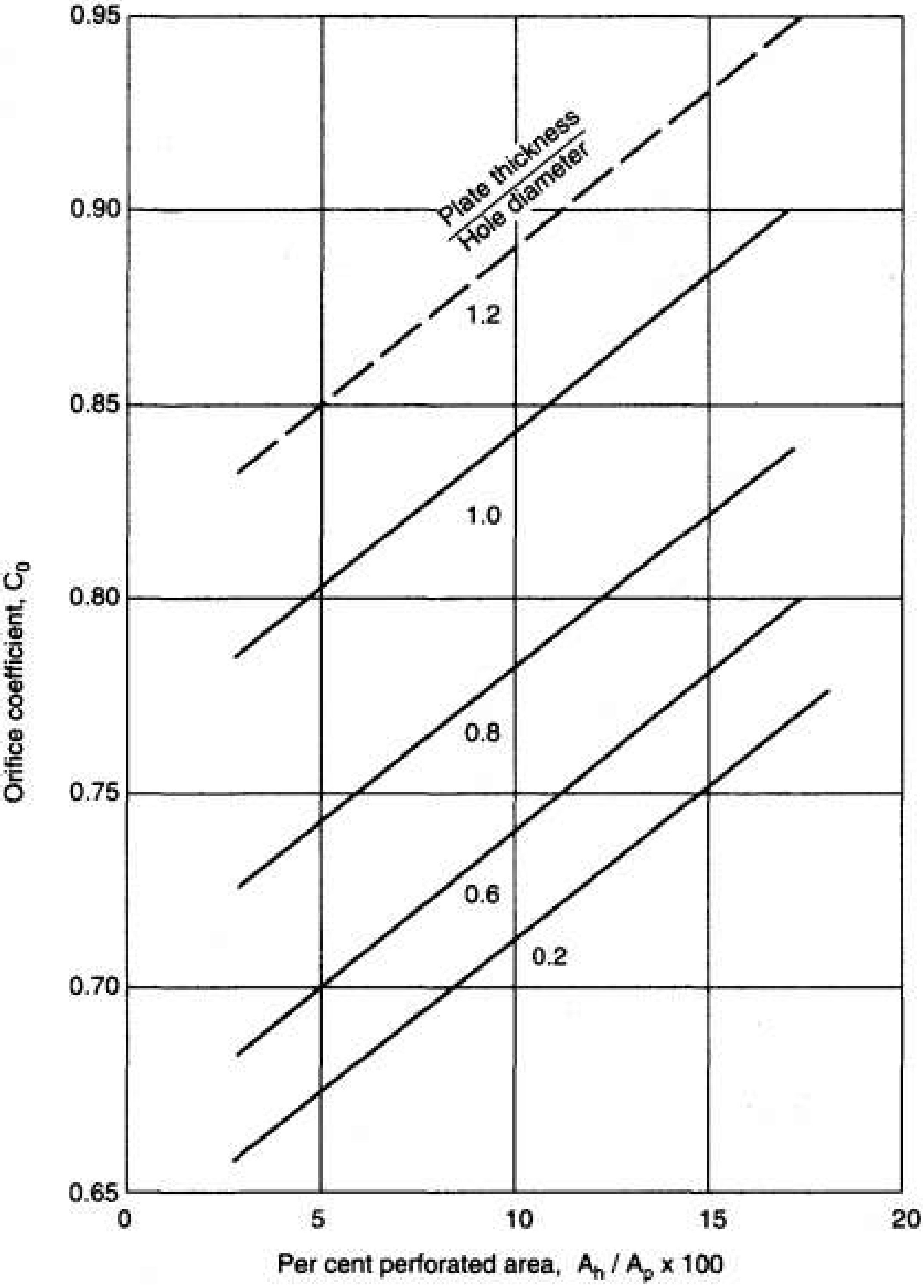
**Appendix J:** Relation between angle subtended by chord,



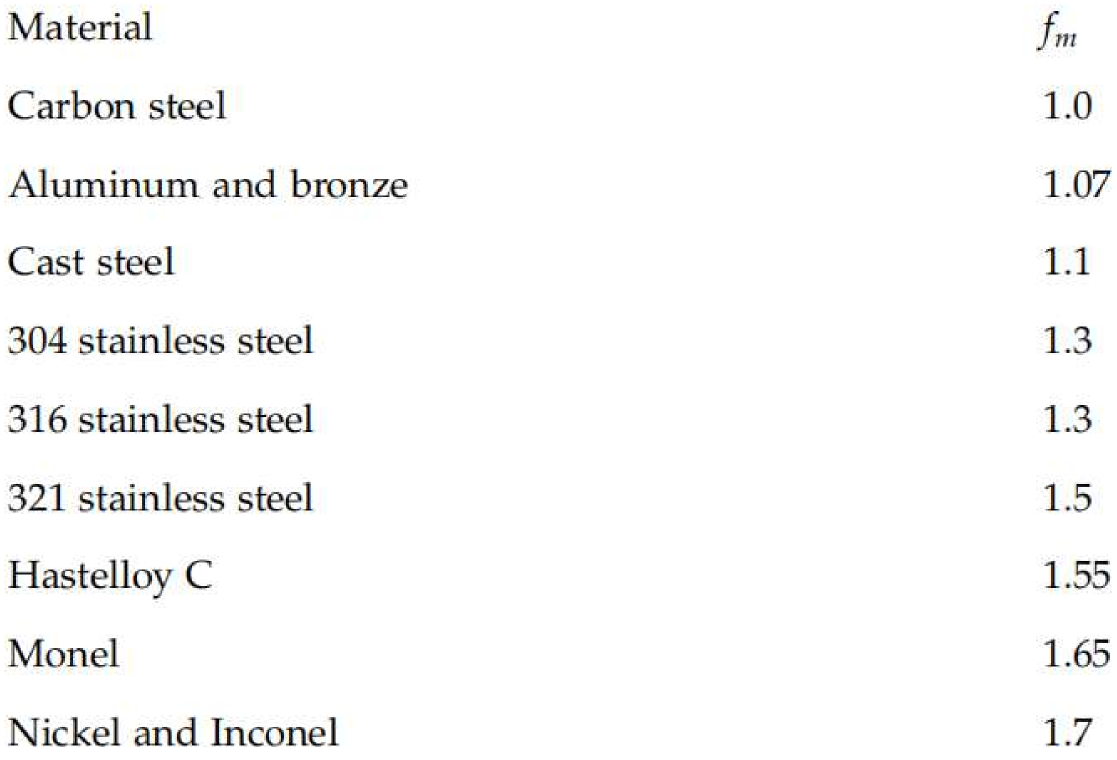
**Appendix K:** Relation between hole area and pitch



**Appendix L:** Discharge coefficient, sieve plates



## **Appendix M:** Materials cost factors, fm, relative to plain carbon steel

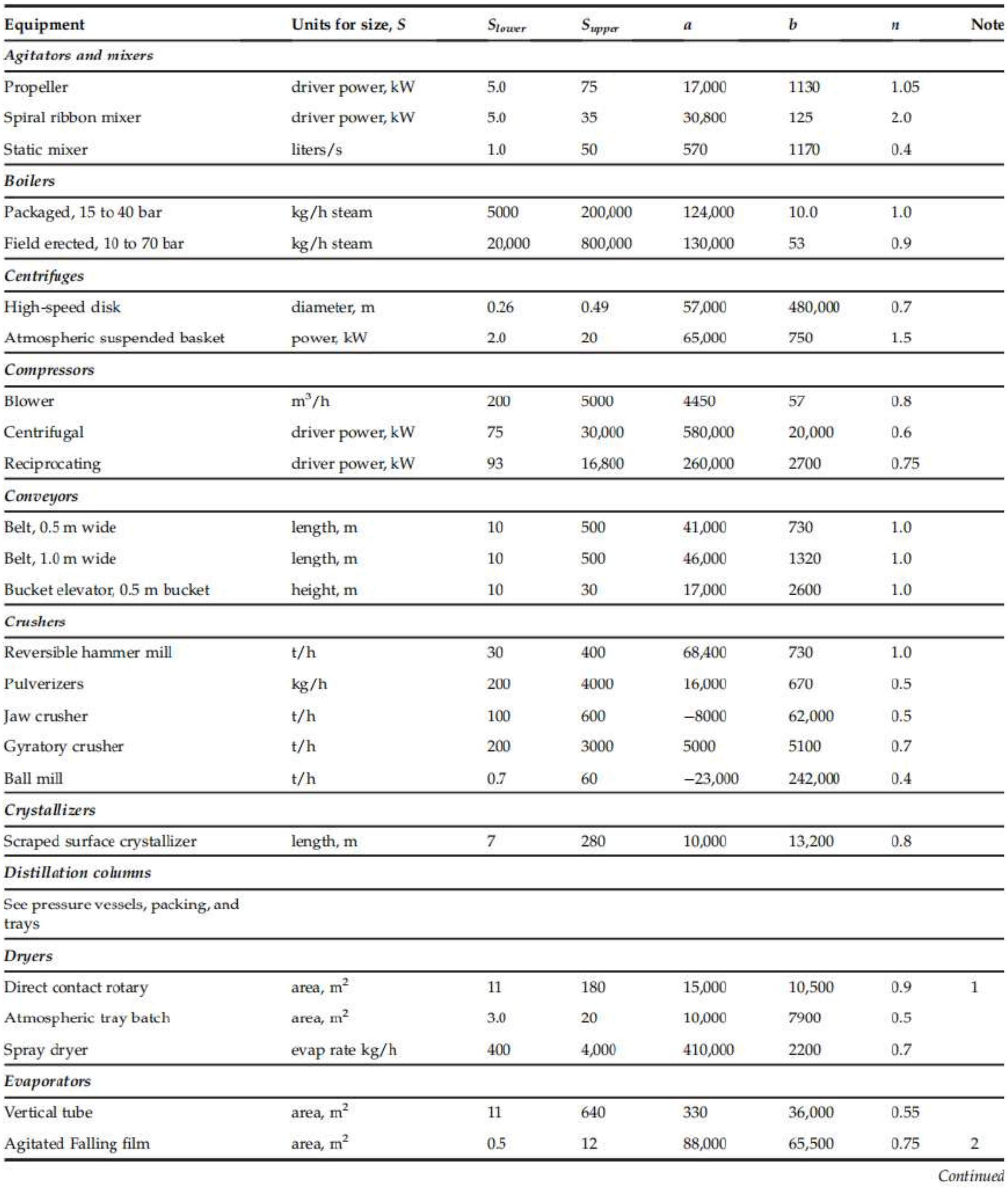


| Material | $f_m$ |
|---|---|
| Carbon steel | 1.0 |
| Aluminum and bronze | 1.07 |
| Cast steel | 1.1 |
| 304 stainless steel | 1.3 |
| 316 stainless steel | 1.3 |
| 321 stainless steel | 1.5 |
| Hastelloy C | 1.55 |
| Monel | 1.65 |
| Nickel and Inconel | 1.7 |

## **Appendix N:** Installation factors proposed by Hand (1958)

| Equipment type | Installation factor |
|---|---|
| Compressors | 2.5 |
| Distillation columns | 4 |
| Fired heaters | 2 |
| Heat exchangers | 3.5 |
| Instruments | 4 |
| Miscellaneous equipment | 2.5 |
| Pressure vessels | 4 |
| Pumps | 4 |

**Appendix O:** Purchased equipment cost for common plant equipment



| Equipment | Units for size, $S$ | $S_{lower}$ | $S_{upper}$ | $a$ | $b$ | $n$ | Note |
|---|---|---|---|---|---|---|---|
| *Agitators and mixers* | | | | | | | |
| Propeller | driver power, kW | 5.0 | 75 | 17,000 | 1130 | 1.05 | |
| Spiral ribbon mixer | driver power, kW | 5.0 | 35 | 30,800 | 125 | 2.0 | |
| Static mixer | liters/s | 1.0 | 50 | 570 | 1170 | 0.4 | |
| *Boilers* | | | | | | | |
| Packaged, 15 to 40 bar | kg/h steam | 5000 | 200,000 | 124,000 | 10.0 | 1.0 | |
| Field erected, 10 to 70 bar | kg/h steam | 20,000 | 800,000 | 130,000 | 53 | 0.9 | |
| *Centrifuges* | | | | | | | |
| High-speed disk | diameter, m | 0.26 | 0.49 | 57,000 | 480,000 | 0.7 | |
| Atmospheric suspended basket | power, kW | 2.0 | 20 | 65,000 | 750 | 1.5 | |
| *Compressors* | | | | | | | |
| Blower | $m^3/h$ | 200 | 5000 | 4450 | 57 | 0.8 | |
| Centrifugal | driver power, kW | 75 | 30,000 | 580,000 | 20,000 | 0.6 | |
| Reciprocating | driver power, kW | 93 | 16,800 | 260,000 | 2700 | 0.75 | |
| *Conveyors* | | | | | | | |
| Belt, 0.5 m wide | length, m | 10 | 500 | 41,000 | 730 | 1.0 | |
| Belt, 1.0 m wide | length, m | 10 | 500 | 46,000 | 1320 | 1.0 | |
| Bucket elevator, 0.5 m bucket | height, m | 10 | 30 | 17,000 | 2600 | 1.0 | |
| *Crushers* | | | | | | | |
| Reversible hammer mill | t/h | 30 | 400 | 68,400 | 730 | 1.0 | |
| Pulverizers | kg/h | 200 | 4000 | 16,000 | 670 | 0.5 | |
| Jaw crusher | t/h | 100 | 600 | −8000 | 62,000 | 0.5 | |
| Gyratory crusher | t/h | 200 | 3000 | 5000 | 5100 | 0.7 | |
| Ball mill | t/h | 0.7 | 60 | −23,000 | 242,000 | 0.4 | |
| *Crystallizers* | | | | | | | |
| Scraped surface crystallizer | length, m | 7 | 280 | 10,000 | 13,200 | 0.8 | |
| *Distillation columns* | | | | | | | |
| See pressure vessels, packing, and trays | | | | | | | |
| *Dryers* | | | | | | | |
| Direct contact rotary | area, $m^2$ | 11 | 180 | 15,000 | 10,500 | 0.9 | 1 |
| Atmospheric tray batch | area, $m^2$ | 3.0 | 20 | 10,000 | 7900 | 0.5 | |
| Spray dryer | evap rate kg/h | 400 | 4,000 | 410,000 | 2200 | 0.7 | |
| *Evaporators* | | | | | | | |
| Vertical tube | area, $m^2$ | 11 | 640 | 330 | 36,000 | 0.55 | |
| Agitated Falling film | area, $m^2$ | 0.5 | 12 | 88,000 | 65,500 | 0.75 | 2 |

*Continued*

| **Equipment** | **Units for size, $S$** | $S_{lower}$ | $S_{upper}$ | $a$ | $b$ | $n$ | **Note** |
|---|---|---|---|---|---|---|---|
| ***Exchangers*** | | | | | | | |
| U-tube shell and tube | area, $m^2$ | 10 | 1000 | 28,000 | 54 | 1.2 | |
| Floating head shell and tube | area, $m^2$ | 10 | 1000 | 32,000 | 70 | 1.2 | |
| Double pipe | area, $m^2$ | 1.0 | 80 | 1900 | 2500 | 1.0 | |
| Thermosiphon reboiler | area, $m^2$ | 10 | 500 | 30,400 | 122 | 1.1 | |
| U-tube Kettle reboiler | area, $m^2$ | 10 | 500 | 29,000 | 400 | 0.9 | |
| Plate and frame | area, $m^2$ | 1.0 | 500 | 1600 | 210 | 0.95 | 2 |
| ***Filters*** | | | | | | | |
| Plate and frame | capacity, $m^3$ | 0.4 | 1.4 | 128,000 | 89,000 | 0.5 | |
| Vacuum drum | area, $m^2$ | 10 | 180 | −73,000 | 93,000 | 0.3 | |
| ***Furnaces*** | | | | | | | |
| Cylindrical | duty, MW | 0.2 | 60 | 80,000 | 109,000 | 0.8 | |
| Box | duty, MW | 30 | 120 | 43,000 | 111,000 | 0.8 | |
| ***Packings*** | | | | | | | |
| 304 ss Raschig rings | $m^3$ | | | 0 | 8000 | 1.0 | |
| Ceramic Intalox saddles | $m^3$ | | | 0 | 2000 | 1.0 | |
| 304 ss pall rings | $m^3$ | | | 0 | 8500 | 1.0 | |
| PVC structured packing | $m^3$ | | | 0 | 5500 | 1.0 | |
| 304 ss structured packing | $m^3$ | | | 0 | 7600 | 1.0 | 3 |
| ***Pressure vessels*** | | | | | | | |
| Vertical, cs | shell mass, kg | 160 | 250,000 | 11,600 | 34 | 0.85 | 4 |
| Horizontal, cs | shell mass, kg | 160 | 50,000 | 10,200 | 31 | 0.85 | 4 |
| Vertical, 304 ss | shell mass, kg | 120 | 250,000 | 17,400 | 79 | 0.85 | 4 |
| Horizontal, 304 ss | shell mass, kg | 120 | 50,000 | 12,800 | 73 | 0.85 | 4 |
| ***Pumps and drivers*** | | | | | | | |
| Single-stage centrifugal | flow liters/s | 0.2 | 126 | 8000 | 240 | 0.9 | |
| Explosion proof motor | power, kW | 1.0 | 2500 | −1100 | 2100 | 0.6 | |
| Condensing steam turbine | power, kW | 100 | 20,000 | −14,000 | 1900 | 0.75 | |
| ***Reactors*** | | | | | | | |
| Jacketed, agitated | volume, $m^3$ | 0.5 | 100 | 61,500 | 32,500 | 0.8 | 2 |
| Jacketed, agitated, glass lined | volume, $m^3$ | 0.5 | 25 | 12,800 | 88,200 | 0.4 | |
| ***Tanks*** | | | | | | | |
| Floating roof | capacity, $m^3$ | 100 | 10,000 | 113,000 | 3250 | 0.65 | |
| Cone roof | capacity, $m^3$ | 10 | 4000 | 5800 | 1600 | 0.7 | |
| ***Trays*** | | | | | | | |
| Sieve trays | diameter, m | 0.5 | 5.0 | 130 | 440 | 1.8 | 5 |
| Valve trays | diameter, m | 0.5 | 5.0 | 210 | 400 | 1.9 | |
| Bubble cap trays | diameter, m | 0.5 | 5.0 | 340 | 640 | 1.9 | |
| ***Utilities*** | | | | | | | |
| Cooling tower and pumps | flow liters/s | 100 | 10,000 | 170,000 | 1500 | 0.9 | 6 |
| Packaged mechanical refrigerator | evaporator duty, kW | 50 | 1,500 | 24,000 | 3500 | 0.9 | |
| Water ion exchange plant | flow $m^3/h$ | 1 | 50 | 14,000 | 6200 | 0.75 | |

# Chapter 15

# References

# REFERENCES

1. Luyben, M.L. and B.D. Tyréus, *An industrial design/control study for the vinyl acetate monomer process.* Computers & Chemical Engineering, 1998. **22**(7-8): p. 867-877.
2. Yan, F.-W., et al., *Vinyl acetate formation in the reaction of acetylene with acetic acid catalyzed by zinc acetate supported on porous carbon spheres.* Russian Journal of Physical Chemistry A, 2010. **84**: p. 796-801.
3. Machida, Y., et al., *Vinyl Acetate Monomer (VAM) Plant Model: A New Benchmark Problem for Control and Operation Study.* IFAC-PapersOnLine, 2016. **49**: p. 533-538.
4. *<chemical-process-design-alexandre.pdf>.*
5. LaBelle, E.V. and H.D. May, *Energy Efficiency and Productivity Enhancement of Microbial Electrosynthesis of Acetate.* Front Microbiol, 2017. **8**: p. 756.
6. Dimian, A.C. and C.S. Bildea, *Chemical process design: Computer-aided case studies*. 2008: John Wiley & Sons.
7. Trotus, I.-T., T. Zimmermann, and F. Schuth, *Catalytic reactions of acetylene: A feedstock for the chemical industry revisited.* Chemical reviews, 2014. **114**(3): p. 1761-1782.
8. Luyben, W.L., *Design and control of a modified vinyl acetate monomer process.* Industrial & engineering chemistry research, 2011. **50**(17): p. 10136-10147.
9. Barroso Rodríguez, P., *Simulación dinámica y control de una planta de producción de Isooctano.* 2011.
10. Cps, C., *Process safety leading and lagging metrics.* Center for Chemical Process Safety. AIChE, New York, http://www. aiche. org/sites/default/files/docs/pages/CCPS. ProcessSafety-Lagging_2011-2-24. pdf (accessed 07.06. 15), 2011.
11. Willey, R.J., D.A. Crowl, and W. Lepkowski, *The Bhopal tragedy: its influence on process and community safety as practiced in the United States.* Journal of loss prevention in the process industries, 2005. **18**(4-6): p. 365-374.
12. Rogers, R.L., B. Broeckmann, and N. Maddison. *Explosion safety document for the ATEX 137 Directive-new name for a fire and explosion hazard assessment?*

in *INSTITUTION OF CHEMICAL ENGINEERS SYMPOSIUM SERIES*. 2003. Institution of Chemical Engineers; 1999.

13. Maguire, S. and C. Hardy, *Organizing processes and the construction of risk: A discursive approach.* Academy of Management Journal, 2013. **56**(1): p. 231-255.
14. Malça, J. and F. Freire, *Life-cycle studies of biodiesel in Europe: A review addressing the variability of results and modeling issues.* Renewable and sustainable energy reviews, 2011. **15**(1): p. 338-351.
15. Cai, H., et al., *Decarbonization potential of on-road fuels and powertrains in the European Union and the United States: a well-to-wheels assessment.* Sustainable Energy & Fuels, 2022. **6**(19): p. 4398-4417.