A Project Report

On

Production of 200 MTPD (73000 MTPY) of Styrene from Ethyl Benzene

B.Sc. Chemical Engineering

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SCHOOL OF CHEMICAL ENGINEERING

Minhaj University Lahore, Pakistan

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This project is submitted to School of Chemical Engineering Minhaj University Lahore, Pakistan.

For the commencement of the requirement for the bachelor's degree in chemical engineering

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بِسْمِ ٱللَّهِ ٱلرَّحْمَٰنِ ٱلرَّحِيمِ

Acknowledgement

All praises be to **Allah**, the lord of all world. It is undeniable that all manifestation of nature bears eloquent testimony to the fact that, **Allah** is the Creator, Maintainer and regulator of the world. He makes laws for the evaluation of things and set them on the path of perfection. Almighty **Allah** who bestows and blesses knowledge, technology, and scientific ingenuity to man through experiment research and remarkable dedication to ponder over the force of nature. In the first place, therefore, we express our utmost thanks to Almighty **Allah** the omnipresent, omnipotent and creator of the world, who has endowed me brain and instable instinct of knowledge.

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CHAPTER 1

INTRODUCTION

1 Introduction

1.1 Introduction:

Styrene was discovered in 1839, by a German druggist Eduard Simon when he isolated a volatile oil from the resin present in the American Sweetgum tree liquidambar styraciflua. He named that oil “styrol” which is currently known as styrene. By further experimenting on his discovery, he found out that when the volatile oil is exposed to air or heat, it continuously converts into a hard, rubber-like substance, which he then named “Styroloxyd” reacting with oxygen this substance is known as polystyrene. By 1845, a German chemist August Hofmann and his student John Blyth determined the empirical formula of styrol which is C_8H_8, they also renamed “Styroloxyd” to “Metastryol” and discovered that it has same empirical formula as styrol.

The modern process for the production of styrene by dehydrogenation of ethyl Benzene was first attained in 1930s. The production of styrene increased rapidly during the second world war near 1940s. At the beginning it was used as a feedstock for synthetic rubber. As the demand for styrene increased and its production started on large scale, ethyl Benzene is then prepared on a colossal scale

Styrene is a colorless oily liquid that evaporates easily and has a sweet smell, although high concentrations have less pleasant odor. It has a melting point at -306 degree Celsius. In the era of world war, we sited an increase in styrene demand as it was used for the manufacturing of synthetic rubber. Styrene has a wide spectrum of applications in producing plastic and synthetic rubber sector. It is prominently used in manufacturing of polystyrene (PS), acrylonitrile-butadiene-styrene (ABS), styrene acrylonitrile (SAN), styrene-butadiene-rubber (SBR) and lattices, polyester resins (UP-resins) and diverse uses like textile auxiliaries, pigment binders, polyester resins, Aromatics and intermediate industries.

1.2 Properties:

TABLE 1-1.1 PHYSICAL PROPERTIES

Properties	Value
Boiling Point at 101.3KPa=1 atm ˚C	145
Freezing Point ˚C	-30.6
Flash point (Fire Point) ˚C	
Tag Open Cup	34.4(34.4)
Cleveland Open-Cup	31.4(34.4)
Auto ignition temperature ˚C	490
Explosive Limits in air %	1.1-6.1
Critical Pressure, P_c, MPa	3.81
Critical temperature ˚C	369.0
Critical Volume V_c	3.55
Refractive index	1.5467

1.3 Scope for Research:

The consumption of styrene and its derivatives was valued at 2.1Million tons in 2022 and the market is about grow to 3.3Million tons by 2030. The Growth rate of this industry is at a compound annual growth rate (CAGR) of 6.0%. The total market worth of styrene production is estimated to be valued at 62.81 Billion USD by 2026. The biggest consumers by volume of styrene and its derivatives are China, Japan, South Korea, Indonesia, India and Australia in Asia-Pacific market. In European Market the consumers are Russia, United Kingdom, France, Germany. In the American market the major consumers are United States and Brazil. In these countries the major consumption reason is their population which is expected to grow up to 5%.

1.4 Market Analysis:

Styrene and its derivatives are widely used in various industries such as packaging, construction, electronics, and consumer goods due to their versatile properties, including light weight, durability, and thermal insulation. The global market for polystyrene and its derivatives has been witnessing steady growth in recent years due to the increasing demand from end-use industries.

1.4.1 Market Overview:

The global polystyrene and its derivatives market size was valued at USD 24.6 billion in 2021 and is expected to reach USD 33.6 billion by 2028, growing at a CAGR of 4.3% from 2021 to 2028. The increasing demand from end-use industries such as packaging, construction, and electronics is the major driver of market growth.

Packaging is the largest application segment of the polystyrene and its derivatives market, accounting for around 55% of the total market share in 2021. The demand for polystyrene-based packaging is increasing due to its properties such as lightweight, durability, and thermal insulation. The increasing demand for packaged food and beverages is expected to boost the growth of the packaging segment.

The construction industry is also a significant application segment of the polystyrene and its derivatives market, accounting for around 20% of the total market share in 2021. Polystyrene-based insulation materials are widely used in the construction industry for their excellent thermal insulation properties. The increasing demand for energy-efficient buildings is expected to boost the growth of the construction segment.

The electronics industry is also a significant application segment of the polystyrene and its derivatives market, accounting for around 15% of the total market share in 2021. Polystyrene-based materials are widely used in the electronics industry for their excellent electrical insulation properties. The increasing demand for electronic devices is expected to boost the growth of the electronics segment.

1.4.2 Geographical Overview:

Asia-Pacific is the largest market for polystyrene and its derivatives, accounting for around 50% of the total market share in 2021. The increasing demand from end-use industries such as packaging, construction, and electronics is the major driver of market growth in the region. China and India are the major consumers of polystyrene and its derivatives in the Asia-Pacific region.

North America is the second-largest market for polystyrene and its derivatives, accounting for around 25% of the total market share in 2021. The increasing demand from end-use industries such as packaging, construction, and electronics is the major driver of market growth in the region. The United States is the major consumer of polystyrene and its derivatives in the North American region.

Europe is the third-largest market for polystyrene and its derivatives, accounting for around 20% of the total market share in 2021. The increasing demand from end-use industries such as packaging, construction, and electronics is the major driver of market growth in the region. Germany, France, and the United Kingdom are the major consumers of polystyrene and its derivatives in the European region.

1.4.3 Key Players:

The global polystyrene and its derivatives market is highly competitive, with the presence of several key players. Some of the key players operating in the market include Styron LLC, Total S.A., Trinseo S.A., Dow Chemical Company, Chevron Phillips Chemical Company LLC, and BASF SE, among others. These players are focusing on product innovation and expansion of their production capacities to meet the increasing demand from end-use industries.

1.4.4 Domestic Market Research:

In 2021, the styrene market in Pakistan experienced a significant increase, reaching $X, up 78% compared to the previous year. This figure represents the total revenue generated by producers and importers, excluding logistics and marketing costs, as well as retailer margins, which will be included in the final price for consumers. The consumption of styrene has also continued to show remarkable growth, reaching its peak level and expected to continue growing in the near future. Approximately X tons of styrene were imported into Pakistan in 2021, representing a 39% increase compared to the previous year. Imports have generally experienced a prominent increase, with the most notable rate of growth recorded in 2018, up 61% compared to the previous year. Imports hit record highs in 2021 and are expected to gradually increase in the near future. In terms of value, styrene imports rose to $X in 2021, with a prominent expansion over the period under review. The main suppliers of styrene imports to Pakistan were Saudi Arabia, Kuwait, and Taiwan (Chinese), together accounting for 66% of total imports, with China, the United States, Indonesia, and the Netherlands lagging behind, accounting for a further 31%. Amongst the main suppliers, Indonesia experienced the most significant growth in terms of purchases, with a compound annual growth rate (CAGR) of +2,459.5% from 2012 to 2021, while purchases for other leading countries experienced more modest growth rates. In terms of value, the largest styrene suppliers to Pakistan were Saudi Arabia, Kuwait, and Taiwan (Chinese), with a combined 69% share of total imports, while China, the United States, Indonesia, and the Netherlands accounted for a further 28%. Indonesia recorded the highest growth rate in the value of imports among the main suppliers over the period under review, with a CAGR of +3,055.7%, while purchases for other leading countries experienced more modest growth rates.

TABLE 1-2 MARKET ANALYSIS

Reporter	Trade Flow	Product Code	Product Description	Year	Partner	Trade Value 1000USD	Quantity	Quantity Unit
Pakistan	Import	290250	styrene	2019		62558.35	5.84978×10^{7}	Kg
Pakistan	Import	290250	styrene	2019	United States	24706.50	2.31752×10^{7}	Kg
Pakistan	Import	290250	styrene	2019	Saudi Arabia	20179.13	1.92316×10^{7}	Kg
Pakistan	Import	290250	styrene	2019	France	10100.52	8.97322×10^{6}	Kg
Pakistan	Import	290250	styrene	2019	Malaysia	3696.96	3.22095×10^{6}	Kg
Pakistan	Import	290250	styrene	2019	Spain	3348.28	3.44978×10^{6}	Kg
Pakistan	Import	290250	styrene	2019	Kuwait	328.52	278880	Kg
Pakistan	Import	290250	styrene	2019	Unspecified	124.86	106930	Kg
Pakistan	Import	290250	styrene	2019	Netherlands	29.35	22000	Kg
Pakistan	Import	290250	styrene	2019	Singapore	21.87	21600	Kg
Pakistan	Import	290250	styrene	2019	Other Asia,	18.93	15200	Kg
Pakistan	Import	290250	styrene	2019	Germany	3.29	2415	Kg
Pakistan	Import	290250	styrene	2019	Korea, Rep.	0.15	60	Kg

1.5 Applications:

Styrene is used on large scale in resins manufacturing, plastics and lattices polymers by continuous and batch mass polymerization or by emulsions, solution and suspension processes. Styrene responds to several initiators like redox initiator systems, free radical initiators, peroxides and ionic initiators. Acrylates, butadiene, maleic anhydride and methacrylate can be reacted with styrene. The (2000) styrene worldwide consumption is about 20×10^{6} metric tons of one year. For wide range of consumer and for the industrial applications, monomer of styrene is used for manufacturing of polymers.

Polymers include:

- Styrene butadiene emulsion polymers
- Unsaturated-polymer resins
- Styrene acrylate emulsion polymers
- polystyrene

1.6 Process Flow Diagram:

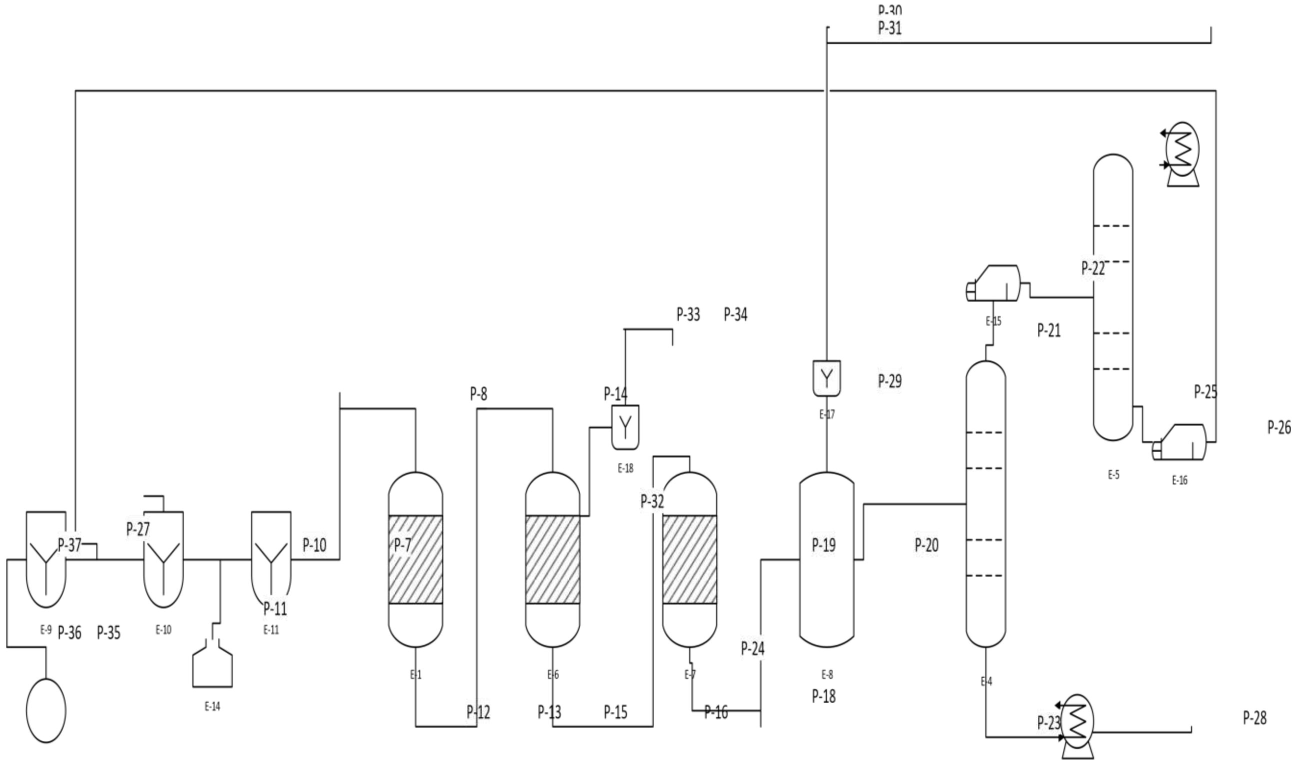

FIGURE 1 PROCESS FLOW DIAGRAM

CHAPTER 2

PROCESS SELECTION

2 Process Selection:

2.1 List of Processes:

Styrene monomer can be produced by the following processes on commercial level.

- Pyrolysis of Petroleum Products.
- Side chain Chlorination of Ethylbenzene.
- Oxidation of Ethylbenzene to Vinyl-Benzene.
- Catalytic dehydrogenation of Ethylbenzene.

2.1.1 Pyrolysis of Petroleum Products:

In this process the products from petroleum recovery is distilled to extract the desired product which is then extractive distilled and the treated with nitric acid. This product is then retreated and washed with water or alkali to gain Vinyl-Benzene monomer.

2.1.2 Side chain Chlorination of Ethylbenzene:

In Side chain Chlorination of Ethyl-Benzene chlorine react with Ethyl-Benzene and form Chlorinated Ethyl-Benzene which is an intermediate this process take place under high temperature which helps the reaction to uniformly take place. This intermediate Chlorinated Ethylbenzene is then reacted with water then this reaction form ethylbenzeldehyde.

2.1.3 Isothermal dehydrogenation of ethyl benzene

Adiabatic dehydrogenation is the most used technology for production of styrene. BASF has been using isothermal dehydrogenation technology for many years to produce styrene at its plants. The basic design of isothermal reactor is like a shell and tube heat exchanger; the reactants flow through the shell side. The diameter of tubes may vary between 1 and 21/2. The tube lengths are approximately 8-10 ft. The largest single shell contains as many as 20,000 – 30,000 tubes and can produce a maximum of 300 million lb. per year styrene. Flue gas a lower heat capacity than the molten salt and must be heated to close to 1,500F to supply the heat required for the ethyl benzene dehydrogenation.

Isothermal dehydrogenation processes have not been used for styrene production. The capital cost of an isothermal reaction system greater than that for an adiabatic system. About isothermal processes, the difficulties over multiples tubes and the mechanical problems associated with circulating a high temperature heating medium.

2.1.4 Adiabatic Dehydrogenation:

Adiabatic dehydrogenation is the worldwide used technology today. Used for commercial styrene production. The dehydrogenation of ethyl benzene to styrene is an **endothermic reaction**. The reaction is carried out with steam. At temperature from 1000 – 1200F and with pressure from 8-15 psig. The steam is added for three reasons: First steam provides heat for reaction. Second the dilution effect of steam lowers the partial pressure of styrene and hydrogen to shift the thermodynamic equilibrium in favors of the decomposition of the ethyl benzene. Finally, the steam reacts with the coke deposited on the catalyst through water-gas shift reaction Thus keeps the catalyst surface available for dehydrogenation the major aromatic by-products from the dehydrogenation of ethyl benzene are Benzene &Toluene.

Conversion and *selectivity* are affected by a number of variables like.

- Temperature
- Pressure
- Steam hydrocarbon ratio
- Space velocity
- Catalyst type

Higher temperature increases the conversion but decrease the selectivity to styrene Both the conversion and styrene selectivity increase with lower reaction pressure Higher steam hydrocarbon ratio the conversion in the reactor is limited to about 40% if no heat is used. When the reactor inlet temperature finally reaches the mechanical design limit. The plant may extend the catalyst life. Almost all catalyst used in commercial ethyl benzene dehydrogenation are made of Iron oxide with potassium oxide and other promoters. The potassium oxide helps to improve the activity by catalyzing the removal of coke from the catalyst.

There are basically two types of catalysts available on the market:

- Those catalyst that gives high styrene selectivity but have lower activities.
- Those catalyst that offers high activity but low selectivity.

Many styrene catalysts also contain a small amount of chromium oxide as a structural stabilizer. The selection of catalyst for commercial styrene production is based on the trade-off raw material versus energy costs.

CHAPTER 3

MATERIAL BALANCE

3 Mass Balance:

3.1 Specifications of the reaction:

Following are the specifications of the reaction and the process which will help us to calculate the total amount of ethyl benzene is required to make 200 metric ton of Styrene per day.

TABLE 3-1 CONVERSATION RATE

Conversion rate of Ethyl Benzene	
Conversion rate of ethyl benzene in reactor 1(R-100)	35%
Conversion rate of ethyl benzene in reactor 1(R-101)	30%
Overall Conversion rate	65%
Selectivity	
Styrene, Hydrogen	95%
Benzene, Ethylene	3%
Toluene, Methane	2%
Molar Ratio	
Super-heated steam/ Ethyl Benzene in reactor 1 (R-100)	6:1
Super-heated steam/ Ethyl Benzene in reactor 1 (R-100)	8:1

Major Reactions Occurring

- ***Reaction#1***

$$\mathrm{C_8H_{10} \rightarrow C_8H_8 + H_2}$$

Ethyl Benzene Styrene Hydrogen

- ***Reaction#2***

$$C_{10}H_{10} + H_2 \rightarrow C_7H_8 + CH_4$$

Ethyl Benzene Hydrogen Toluene Methane

- ***Reaction#3***

$$C_8H_{10} \rightarrow C_6H_6 + C_2H_4$$

Ethyl Benzene Benzene Ethylene

- ***Reaction#4***

$$H_2 + O_2 \rightarrow H_2O$$

3.2 Feed mass calculation:

Basis: 73000 metric ton per year production of Styrene.

Styrene to be produced =73000$\frac{Ton}{Year}$

Styrene in product = $\frac{73000Kg \times 1000}{365 \times 24 \times 104.15 g/mol}$

Styrene in product = 80.0128Kmol/hr.

As we know Conversion rate of the reaction is 65%,

Ethyl Benzene required to make Styrene = $\frac{80.0128 kmol/hr.}{0.65}$

Ethyl Benzene required to make Styrene = 123.0966Kmol/hr.

As we know the Selectivity of this reaction is 95%

Ethyl Benzene Required = $\frac{123.0966 kmol/hr.}{0.95}$

Ethyl Benzene Required = 129.5754kmol/hr.

The separator which we are going to use at this site have an efficiency of 98%

The Styrene Column which we are going to use at this site have an efficiency of 99.7%

Ethyl Benzene required = $\frac{129.5754 kmol/hr.}{0.98 \times 99.7}$

Ethyl Benzene required = 132.5562Kmol/hr.

As we know that the selectivity for the production of Toluene and Methane as side reaction is 2%

The mole of Toluene to be produced in this reaction = 132.5562Kmol/hr. ×0.65×0.02

The mole of Toluene to be produced in this reaction = 1.7232Kmol/hr.

The mole of Methane to be produced in this reaction = 132.5562Kmol/hr. ×0.65×0.02

The mole of Methane to be produced in this reaction = 1.7232Kmol/hr.

As we know that the selectivity for the production of Benzene and Ethylene as side reaction is 3%

The mole of Ethylene to be produced in this reaction = 132.5562Kmol/hr. ×0.65×0.03

The mole of Ethylene to be produced in this reaction = 2.5848Kmol/hr.

The mole of Ethylene to be produced in this reaction = 132.5562Kmol/hr. ×0.65×0.03

The mole of Ethylene to be produced in this reaction = 2.5848Kmol/hr.

3.3 Balance on Reactor: (R-100):

Basis: 132.5562 Kmol/hr.

Ethylbenzene Consume (overall)= 132.5562 × 0.35

=46.3947 Kmol/hr.

Using Selectivity:

Styrene Formed = 46.3947×0.95 = 44.0750Kmol/hr.

Hydrogen Formed=46.3947×0.95= 44.0750Kmol/hr.

Toluene Formed:

Toluene Formed= 2% Styrene Formed

=0.02×44.0750Kmol/hr.

=0.8815Kmol/hr.

Methane Formed = 2% Styrene Formed

=0.02×44.0750Kmol/hr.

=0.8815Kmol/hr.

Benzene Formed:

Benzene formed= 3% Styrene Formed

=0.03×44.0750Kmol/hr.

=1.3223Kmol/hr.

Ethylene Formed:

Ethylene formed= 3% Styrene Formed

=0.03×44.0750Kmol/hr.

=1.3223Kmol/hr.

The total mass flow rate of Product at the outlet of the reactor (R-100) = 44.0750Kmol/hr. + 2(0.8815Kmol/hr.) +2(1.3223Kmol/hr.)

=48.4826 Kmol/hr.

Total Ethyl Benzene left after reaction consumed = 132.5562Kmol/hr. – 48.4826Kmol/hr.

Total Ethyl Benzene left after reaction consumed = 84.0736Kmol/hr.

3.4 Balance on Reactor: (R-101)

Basis: 84.0736Kmol/hr.

Ethylbenzene Consume (overall)= 132.5562 × 0.30

=39.7669 Kmol/hr.

Using Selectivity:

Styrene Formed = 39.7669×0.95 =37.7786 Kmol/hr.

Hydrogen Formed=39.7669×0.95= 37.7786Kmol/hr.

Toluene Formed:

Toluene Formed= 2% Styrene Formed

=0.02×37.7786Kmol/hr.

=0.7556Kmol/hr.

Methane Formed = 2% Styrene Formed

=0.02×37.7786Kmol/hr.

=0.7556Kmol/hr.

Benzene Formed:

Benzene formed= 3% Styrene Formed

=0.03×37.7786Kmol/hr.

=1.1334Kmol/hr.

Ethylene Formed:

Ethylene formed= 3% Styrene Formed

=0.03×37.7786Kmol/hr.

=1.1334Kmol/hr.

The total mass flow rate of Product at the outlet of the reactor (R-100) = 37.7786Kmol/hr. + 2(0.7556Kmol/hr.) +2(1.1334Kmol/hr.)

= 41.5566Kmol/hr.

Total Ethyl Benzene left after reaction consumed = 132.5562Kmol/hr. – 48.4826Kmol/hr. – 41.5566 Kmol/hr.

Total Ethyl Benzene left after reaction consumed = 42.5170Kmol/hr.

3.5 Balance around Separator:

Overall, Balance:

u = Wastewater

v = Gases

w = Styrene

x = Ethylbenzene

y = Toluene

z = Benzene

Steam added to first reactor = Moles of Ethylbenzene ×6

Steam added to first reactor = 132.5562Kmol/hr. × 6

Steam added to first reactor = 795.3372Kmol/hr.

Steam added to the second reactor = moles of ethylbenzene ×8

As, the conversion rate is 35% so,

Steam added to the second reactor =132.5562Kmol/hr.-(0.35× 132.5562Kmol/hr.) × 8

Steam added to the second reactor = 238.6012Kmol/hr.

Total Steam added = 1033.9384Kmol/hr.

Styrene in the separator = $\frac{81.8536 Kmol/hr}{0.997 \times 0.98}$

Styrene in the Separator = 80.0128Kmol/hr.

Ethylbenzene in Separator = $\frac{42.5170 Kmol/hr}{0.997 \times 0.98}$

Ethylbenzene in Separator = 43.5152Kmol/hr.

Toluene in Separator = $\frac{1.6371 Kmol/hr}{0.98}$

Toluene in separator = 1.6705Kmol/hr.

Methane in Separator = $\frac{1.6371 Kmol/hr}{0.98}$

Methane in Separator = 1.6705Kmol/hr.

Hydrogen at the inlet of Separator = 80.0128 – 2(1.6371)

Moles of Hydrogen = 76.7386Kmol/hr.

Benzene in Separator = $\frac{2.0402 Kmol/hr}{0.98}$

Benzene in Separator = 2.5058Kmol/hr.

Ethylene in the Separator = $\frac{2.0402 Kmol/hr}{0.98}$

Ethylene in the separator = 2.5058Kmol/hr.

Totalfeedofseparator=A=795.3372Kmol/hr.+1033.9384Kmol/hr.+80.0128Kmol/hr.+43.5152 Kmol/hr.+1.6705Kmol/hr.+1.6705Kmol/hr.+76.7386Kmol/hr.+2.5058Kmol/hr.+2.5058Kmol /hr.

Total feed of Separator = A = 2037.8948Kmol/hr.

Total outlet of the separator = A=B+C+D

A = B+C+D

Were,

B = Steam to be Separator =1829.2756Kmol/hr.

C = Product to be Separated=?

D = Gases to be Separator =80.9149Kmol/hr.

2039.7445Kmol/hr.=1829.2756Kmol/hr.+C+80.9149Kmol/hr.

C = 2037.8948Kmol/hr.-1829.2756Kmol/hr.-80.9149Kmol/hr.

C=127.7043Kmol/hr.

3.6 Balance on Styrene Column (T-101)

Let,

x= Ethylene Benzene

w= Styrene

y=Toluene

z=Benzene

Overall, Balance:

A=B+C

Styrene Balance:

wA= wB+wC

Ethylbenzene Balance:

xA=xB+xC

Toluene Balance:

yA=yB+yC

Benzene Balance:

zA=zB+zC

At the inlet of distillation Column:

Styrene in product = $\frac{73000Kg \times 1000}{365\times 24\times 104.15g/mol}$ =80.0128Kmol/hr.

Unreacted Ethylbenzene = 43.1882Kmol/hr.

Moles Produced of toluene = 0.65×0.02×123.0966Kmol/hr.

Moles Produced of toluene =1.6003Kmol/hr.

Moles Produced of Benzene = 0.65×0.03×123.0966Kmol/hr.

Moles Produced of Benzene = 2.4004Kmol/hr.

This means that A which is the inlet of the column = Moles of Toluene + Moles of Benzene

A = B+C

A=2.4004Kmol/hr.+1.6003Kmol/hr.

A= 4.0007Kmol/hr.

3.7 Balance on Distillation Column (T-100)

Overall, Balance:

Let,

x= Ethylene Benzene

w= Styrene

Overall, Balance:

A=B+C

Styrene Balance:

wA= wB+wC

Ethylbenzene Balance:

xA=xB+xC

Styrene in product = $\frac{73000Kg \times 1000}{365 \times 24 \times 104.15 g/mol}$ =80.0128Kmol/hr.

The purity of styrene at the bottom of the column is 99.7% and the purity of ethylbenzene at the top of column is 99% so, as the conversion rate is 65% then the inlet stream of the column has 65% styrene and 35% Ethylbenzene.

A= B+80.0128Kmol/hr.

xA=xB+x(80.0128Kmol/hr.)

0.65A=0.1(B) + 0.997(80.0128Kmol/hr.)

0.65(A)=0.1(B) + 79.7728Kmol/hr.

Using the equations

0.65(B+80.0128Kmol/hr.) = 0.1(B) + 79.7728Kmol/hr.

0.65B + 52.0083kmol/hr. = 0.1B + 79.7728Kmol/hr.

B (0.65-0.1) = 79.7728Kmol/hr. – 52.0083Kmol/hr.

0.64B= 27.7645Kmol/hr.

B= $\frac{27.7645}{0.64}$ Kmol/hr.

B=43.3820Kmol/hr.

Now putting the value of B in equation 1

A=43.3820Kmol/hr. + 80.0128Kmol/hr.

A = 123.3948Kmol/hr.

Now the total flow rate will be multiplied by the concentration to find the respective specie

Styrene at outlet = 0.65×123.3948Kmol/hr.

Styrene at outlet = 80.2066Kmol/hr.

Ethylbenzene at outlet = 0.35 ×123.3948Kmol/hr.

Ethylbenzene at outlet = 43.1882Kmol/hr.

CHAPTER 4

ENERGY BALANCE

4 Energy Balance

4.1 Energy Balance around Mixing Point: (M-101)

At first, we have to find out the temperature of Mixer 1;

$Q=mC_P\Delta T$

Were,

Q is Heat energy

m is mass flow rate

C_p is specific heat capacity.

ΔT is the change in temperature.

Following is the table enlisting the heat capacities of different components of the process

TABLE 4-1 HEAT CAPACITIES OF SPECIES

Chemical Name	A $({}^{KJ}/_{Kmol})$	B $({}^{KJ}/_{Kmol})$	C $({}^{KJ}/_{Kmol})$	D $({}^{KJ}/_{Kmol})$	Temperature (K)
Ethyl Benzene	-20.527	5.9578×10^{-1}	-3.084×10^{-4}	3.5721×10^{-8}	200-1500
Styrene	77.201	5.67×10^{-2}	6.4793×10^{-4}	-6.987×10^{-7}	100-1500
Toluene	-24.097	5.2187×10^{-1}	-2.982×10^{-4}	6.1220×10^{-8}	200-1500
Methane	34.942	-3.9957×10^{-2}	1.9184×10^{-4}	-1.530×10^{-7}	50-1500
Benzene	-31.368	4.746×10^{-1}	-3.113×10^{-4}	8.5237×10^{-8}	200-1500
Ethylene	32.083	-1.4831×10^{-2}	2.4774×10^{-4}	-2.376×10^{-7}	60-1500
Hydrogen	25.399	2.0178×10^{-2}	-3.854×10^{-5}	3.1880×10^{-8}	250-1500
Water	33.933	-8.4186×10^{-3}	2.9906×10^{-5}	-1.782×10^{-8}	100-1500

$C_P\Delta T$ on fresh ethylbenzene = $-20.527{}^{KJ}/_{Kmol} \times (293K-298K) + (5.9578\times\frac{10^{-1}}{2})\,{}^{KJ}/_{Kmol} \times (293^2K-298^2K) + (-3.084\times\frac{10^{-4}}{3})\,{}^{KJ}/_{Kmol} \times (293^3K-298^3K) + (3.5721\times\frac{10^{-8}}{4})\,{}^{KJ}/_{Kmol} \times (293^4K-298^4K)$

$C_P\Delta T$ on fresh ethylbenzene = $-916.8898{}^{KJ}/_{Kmol}$

$C_P\Delta T$ on recycled ethylbenzene = $-20.527\,{}^{KJ}/_{Kmol} \times (403K-298K) + (5.9578\times\frac{10^{-1}}{2})\,{}^{KJ}/_{Kmol} \times (403^2K-298^2K) + (-3.084\times\frac{10^{-4}}{3})\,{}^{KJ}/_{Kmol} \times (403^3K-298^3K) + (3.5721\times\frac{10^{-8}}{4})\,{}^{KJ}/_{Kmol} \times (403^4K-298^4K)$

$C_P\Delta T$ on recycled ethylbenzene = $16093.2208\,{}^{KJ}/_{Kmol}$

$Q_{inlet} = mC_P\Delta T$ on fresh ethylbenzene + $mC_P\Delta T$ on recycled ethylbenzene

$Q_{inlet} = 79.9084 Kmol/hr. \times (-916.8898\,{}^{KJ}/_{Kmol}) + 43.1882 Kmol/hr. \times (16093.2208\,{}^{KJ}/_{Kmol})$

$Q_{inlet} = 621770.0417 KJ/hr.$

4.1.1 Heat outlet:

$C_P\Delta T$ on product ethylbenzene = $-20.527\,{}^{KJ}/_{Kmol} \times (333.88K-298K) + (5.9578\times\frac{10^{-1}}{2})\,{}^{KJ}/_{Kmol} \times (333.88K^2-298^2K) + (-3.084\times\frac{10^{-4}}{3})\,{}^{KJ}/_{Kmol} \times (333.88K^3-298^3K) + (3.5721\times\frac{10^{-8}}{4})\,{}^{KJ}/_{Kmol} \times (333.88^4-298^4K)$

$C_P\Delta T$ on product ethylbenzene = 4952.0463KJ/Kmol

$Q_{outlet} = mC_P\Delta T$

$Q_{outlet} = 123.0966 Kmol/hr. \times 4952.0463 KJ/Kmol$

$Q_{outlet} = 621557.5017 KJ/hr.$

4.2 Energy Balance on Mixer (M-2)

Steam is added to mixer before first reactor = moles of ethylbenzene × 6

Steam is added to the mixer before first reactor = 123.0966Kmol/hr. × 6 = 738.5796Kmol/hr.

Heat at the inlet:

Ethylbenzene temperature is 773K and 26psi at the inlet of the mixer

So, the value of $C_P\Delta T$ will be found

$C_p\Delta T = -20.527(773-298) +5.9578 \frac{10^{-1}}{2} (773^2-298^2)+(-3.0849 \frac{10^{-4}}{3})(773^3-298^3)+(3.5721\frac{10^{-8}}{4})(773^4-298^4)$

$C_p\Delta T$ = 100136.9155KJ/Kmol

$Q_{E.B}$ = 123.0966Kmol/hr.×100136.9155KJ/Kmol

$Q_{E.B}$ = 12326513.83KJ/hr.

Steam enters at 770˚C (1043K) and the pressure is 14bar

Enthalpy at the inlet of the mixer = h = 73603.0506KJ/Kmol

$Q_{Steam} = m\times h$

Q_{Steam} = 738.5796Kmol/hr.×73603.0506KJ/Kmol

Q_{Steam} = 54361711.67KJ/hr.

Heat outlet:

$Q_{outlet} =(m_1+m_2)(C_p)(\Delta T)$

$Q_{outlet} =$ 66685724.3KJ/hr.

4.3 Reactor Energy Balance (R-100):

4.3.1 Energy balance on inlet:

Heat energy at the inlet of foirst reactor on Ethylbenzene.

$C_p\Delta T = -20.527(908-298) +5.9578 \frac{10^{-1}}{2} (908^2-298^2)+(-3.0849 \frac{10^{-4}}{3})(908^3-298^3)+3.5721\frac{10^{-8}}{4}(908^4-298^4)$

$C_p\Delta T$ = 138365.4625KJ/Kmol

$Q = mC_p\Delta T$

Q = 123.0966Kmol/hr.× 138365.4625KJ/Kmol

Q = 17032317.99KJ/hr.

4.3.2 Energy Balance on the outlet of the first reactor:

Energy Balance on Ethylbenzene

$C_p\Delta T = -20.527(838-298) + 5.9578\ \frac{10^{-1}}{2}\ (838^2-298^2) + (-3.0849\ \frac{10^{-4}}{3}\ )(838^3-298^3) + 3.5721\frac{10^{-8}}{4}(838^4-298^4)$

$C_p\Delta T = 118195.0911$KJ/Kmol

$Q_{E.B} = mC_p\Delta T$

$Q_{E.B}$ =79.9084Kmol/hr. ×118195.0911KJ/Kmol

$Q_{E.B}$ = 9444780.618KJ/hr.

Energy balance on Styrene

$Cp\Delta T = 77.201\times\ (838-298) + 5.67\ \frac{10^{-2}}{2}\ (8382-2982) + 6.4793\times\ \frac{10^{-4}}{3}\ (8383-2983) - (6.987\times\frac{10^{-7}}{4})(8384-2984)$

$C_p\Delta T = 1188142.013$KJ/Kmol

$Q_{Styrene} = mC_p\Delta T$

$Q_{Styrene} =$ 44.0750Kmol/hr. × 1188142.013KJ/Kmol

$Q_{Styrene}$ = 52364359.22KJ/hr.

Energy balance on Toluene

$Cp\Delta T = Cp\Delta T = 24.097(838-298) + 5.2187\frac{10^{-1}}{2}(8382-2982) - (2.9827\frac{10^{-4}}{3})(8383-2983) + 6.1220\frac{10^{-8}}{4}(8384-2984)$

$C_p\Delta T = 124629.6665$KJ/Kmol

$Q_{Toluene} = mC_p\Delta T$

$Q_{Toluene}$ =0.8815Kmol/hr. ×124629.6665KJ/Kmol

$Q_{Toluene}$ = 109861.0510KJ/hr.

Energy Balance on Benzene

$C_p\Delta T = -31.368(838-298) + 4.7460\ \frac{10^{-1}}{2}\ (838^2-298^2) - (3.1137\ \frac{10^{-4}}{3}\ )(838^3-298^3) + 8.5237\frac{10^{-8}}{4}(838^4-298^4)$

$C_p\Delta T$ = 80639.3970KJ/Kmol

Q $_{\text{Benzene}}$ = $mC_p\Delta T$

Q $_{\text{Benzene}}$ =1.3223Kmol/hr. ×80639.39KJ/Kmol

Q $_{\text{Benzene}}$ = 106629.4654KJ/hr.

Energy Balance on Ethylene

$C_p\Delta T = 32.083(838\text{-}298)\ -1.4831\frac{10^{-2}}{2}(838^2\text{-}298^2) - (2.4774\frac{10^{-4}}{3})(838^3\text{-}298^3)\ -2.3766\frac{10^{-7}}{4}(838^4\text{-}298^4)$

$C_p\Delta T$ = 30355.458KJ/Kmol

Q $_{\text{Ethylene}}$ = $mC_p\Delta T$

Q $_{\text{Ethylene}}$ =1.3223Kmol/hr. ×30355.458KJ/Kmol

Q $_{\text{Ethylene}}$ = 40139.0221KJ/hr.

Energy Balance at Methane

$C_p\Delta T = 34.942(838\text{-}298)\ -3.9957\frac{10^{-1}}{2}(838^2\text{-}298^2)\ +(1.9184\frac{10^{-4}}{3})(838^3\text{-}298^3)\ -1.5303\frac{10^{-7}}{4}(838^4\text{-}298^4)$

$C_p\Delta T$ = 23987.3221KJ/Kmol

Q $_{\text{Methane}}$ = $mC_p\Delta T$

Q $_{\text{Methane}}$ =0.8815Kmol/hr. ×23987.3221KJ/Kmol

Q $_{\text{Methane}}$ = 21144.8244KJ/hr.

Energy Balance on Hydrogen:

$C_p\Delta T = 25.399(838\text{-}298)\ +2.0178\frac{10^{-2}}{2}(838^2\text{-}298^2)\ -3.8549(\frac{10^{-5}}{3})(838^3\text{-}298^3)\ +3.1880\frac{10^{-8}}{4}(838^4\text{-}298^4)$

$C_p\Delta T$ = 16550.2521KJ/Kmol

Q $_{\text{Hydrogen}}$ = $mC_p\Delta T$

Q $_{\text{Hydrogen}}$ =39.6684Kmol/hr. ×16550.2521KJ/Kmol

Q_{Hydrogen} = 656522.0204KJ/hr.

4.4 Energy Balance on the Reactor (R-101)

4.4.1 Energy balance on inlet:

Energy Balance on Ethylbenzene

$$C_p\Delta T = -20.527(908-298) + 5.9578\ \frac{10^{-1}}{2}\ (908^2-298^2) + (-3.0849\ \frac{10^{-4}}{3}\ )(908^3-298^3) + 3.5721\frac{10^{-8}}{4}(908^4-298^4)$$

$C_p\Delta T$ = 138365.4625KJ/Kmol

$Q_{E.B} = mC_p\Delta T$

$Q_{E.B}$ = 79.9084Kmol/hr.× 138365.4625KJ/Kmol

$Q_{E.B}$ = 11056562.72KJ/hr.

Energy balance on Styrene

$$Cp\Delta T = 77.201\times\ (908-298) + 5.67\ \frac{10^{-2}}{2}\ (908-2982) + 6.4793\times\ \frac{10^{-4}}{3}\ (908-2983) - (6.987\times\frac{10^{-7}}{4})(908-2984)$$

$C_p\Delta T$ = 106559.8342KJ/Kmol

$Q_{\text{Styrene}} = mC_p\Delta T$

Q_{Styrene} = 44.0750Kmol/hr. ×106559.8342KJ/Kmol

Q_{Styrene} = 4696624.692KJ/hr.

Energy balance on Hydrogen

$$C_p\Delta T = 25.399(908-298) + 2.0178\frac{10^{-2}}{2}(908^2-298^2) - 3.8549(\frac{10^{-5}}{3})(908^3-298^3) + 3.1880\frac{10^{-8}}{4}(908^4-298^4)$$

$C_p\Delta T$ = 18990.7628KJ/Kmol

$Q_{\text{Hydrogen}} = mC_p\Delta T$

Q_{Hydrogen} =39.6684Kmol/hr. ×18990.7628KJ/Kmol

Q_{Hydrogen} = 753333.1751KJ/hr.

Energy balance on Toluene

$C_p\Delta T = C_p\Delta T = 24.097(908\text{-}298) + 5.2187\frac{10^{-1}}{2}(908\text{-}298) - (2.9827\frac{10^{-4}}{3})(908\text{-}298) + 6.1220\frac{10^{-8}}{4}(908\text{-}298)$

$C_p\Delta T$ = 115744.47KJ/Kmol

$Q_{Styrene} = mC_p\Delta T$

$Q_{Toluene}$ = 0.8815Kmol/hr. × 115744.47KJ/Kmol

$Q_{Toluene}$ = 102028.7503KJ/hr.

Energy balance on Benzene

$C_p\Delta T = -31.368(908\text{-}298) + 4.7460\frac{10^{-1}}{2}(908^2\text{-}298^2) - (3.1137\frac{10^{-4}}{3})(908^3\text{-}298^3) + 8.5237\frac{10^{-8}}{4}(908^4\text{-}298^4)$

$C_p\Delta T$ = 94802.439KJ/Kmol

$Q_{Benzene} = m C_p \Delta T$

$Q_{Benzene}$ =1.3223Kmol/hr. ×94802.439KJ/Kmol

$Q_{Benzene}$ = 125357.2651KJ/hr.

Energy balance on Methane

$C_p\Delta T = 34.942(908\text{-}298) - 3.9957\frac{10^{-1}}{2}(908^2\text{-}298^2) + (1.9184\frac{10^{-4}}{3})(908^3\text{-}298^3) - 1.5303\frac{10^{-7}}{4}(908^4\text{-}298^4)$

$C_p\Delta T$ = 27092.82KJ/Kmol

$Q_{Methane} = mC_p\Delta T$

$Q_{Methane}$ =0.8815Kmol/hr. ×27092.82KJ/Kmol

$Q_{Methane}$ = 23882.3208KJ/hr.

Energy balance on Ethylene

$C_p\Delta T = 32.083(908-298) -1.4831\frac{10^{-2}}{2}(908^2-298^2) - (2.4774\frac{10^{-4}}{3})(908^3-298^3) -2.3766\frac{10^{-7}}{4}(908^4-298^4)$

$C_p\Delta T$ = 33832.2KJ/Kmol

$Q_{\text{Ethylene}} = mC_p\Delta T$

Q_{Ethylene} =1.3223Kmol/hr. ×33832.2KJ/Kmol

Q_{Ethylene} = 44736.3181KJ/hr.

4.4.2 Energy Balance on the outlet of the Second reactor:

4.4.2.1 Energy Balance on Ethylbenzene

$C_p\Delta T = -20.527(843-298) +5.9578 \frac{10^{-1}}{2} (843^2-298^2) +(-3.0849 \frac{10^{-4}}{3})(843^3-298^3) +3.5721\frac{10^{-8}}{4}(843^4-298^4)$

$C_p\Delta T$ = 119611.9KJ/Kmol

$Q_{E.B} = mC_p\Delta T$

$Q_{E.B}$ =46.3947Kmol/hr. ×118195.0911KJ/Kmol

$Q_{E.B}$ = 5483625.793KJ/hr.

4.4.2.2 Energy balance on Styrene

$Cp\Delta T = 77.201\times (843-298) +5.67 \frac{10^{-2}}{2} (843-2982) +6.4793\times \frac{10^{-4}}{3} (843-2983) -(6.987\times\frac{10^{-7}}{4})(843-2984)$

$C_p\Delta T$ = 96537.8KJ/Kmol

$Q_{\text{Styrene}} = mC_p\Delta T$

Q_{Styrene} = 81.8536Kmol/hr. × 96537.8KJ/Kmol

Q_{Styrene} = 7901966.466KJ/hr.

4.4.2.3 Energy balance on Toluene

$Cp\Delta T = Cp\Delta T = 24.097(843\text{-}298) + 5.2187\,\frac{10^{-1}}{2}\,(843\text{-}2982) - (2.9827\,\frac{10^{-4}}{3})(843\text{-}2983) + 6.1220\frac{10^{-8}}{4}(843\text{-}298)$

$C_p\Delta T = 99805.77$KJ/Kmol

$Q_{Toluene} = mC_p\Delta T$

$Q_{Toluene} = 1.6371$Kmol/hr. ×99805.77KJ/Kmol

$Q_{Toluene} = 163392.0261$KJ/hr.

4.4.2.4 Energy Balance on Benzene

$C_p\Delta T = -31.368(843\text{-}298) + 4.7460\,\frac{10^{-1}}{2}\,(843^2\text{-}298^2) - (3.1137\,\frac{10^{-4}}{3})(843^3\text{-}298^3) + 8.5237\frac{10^{-8}}{4}(843^4\text{-}298^4)$

$C_p\Delta T = 81630.3$KJ/Kmol

$Q_{Benzene} = mC_p\Delta T$

$Q_{Benzene} = 2.4557$Kmol/hr. ×81630.3KJ/Kmol

$Q_{Benzene} = 200459.5277$KJ/hr.

4.4.2.5 Energy Balance on Ethylene

$C_p\Delta T = 32.083(843\text{-}298) - 1.4831\frac{10^{-2}}{2}(843^2\text{-}298^2) - (2.4774\frac{10^{-4}}{3})(843^3\text{-}298^3) - 2.3766\frac{10^{-7}}{4}(843^4\text{-}298^4)$

$C_p\Delta T = 30623$KJ/Kmol

$Q_{Ethylene} = mC_p\Delta T$

$Q_{Ethylene} = 2.4557$Kmol/hr. ×30623KJ/Kmol

$Q_{Ethylene} = 75200.9011$KJ/hr.

4.4.2.6 Energy Balance at Methane

$C_p\Delta T = 34.942(843-298) -3.9957\frac{10^{-1}}{2}(843^2-298^2) +(1.9184\frac{10^{-4}}{3})(843^3-298^3) -1.5303\frac{10^{-7}}{4}(843^4-298^4)$

$C_p\Delta T = 24217$KJ/Kmol

$Q_{Methane} = mC_p\Delta T$

$Q_{Methane} =1.6371$Kmol/hr. ×24217KJ/Kmol

$Q_{Methane} =39645.6507$ KJ/hr.

4.4.2.7 Energy Balance on Hydrogen:

$C_p\Delta T = 25.399(843-298) +2.0178\frac{10^{-2}}{2}(843^2-298^2) -3.8549(\frac{10^{-5}}{3})(843^3-298^3) +3.1880\frac{10^{-8}}{4}(838^4-298^4)$

$C_p\Delta T = 16720$KJ/Kmol

$Q_{Hydrogen} = mC_p\Delta T$

$Q_{Hydrogen} =73.669$Kmol/hr. ×16720KJ/Kmol

$Q_{Hydrogen} = 1231745.680$KJ/hr.

4.5 Energy Balance around (T-100):

From material balance, for column T-101, the mole fractions are as follows.

Components	Distillate (M)	Bottom (L)
Ethyl benzene	0.92	0.02
Styrene	0.02	0.98
Toluene	0.04	
Benzene	0.02	

Total Moles at inlet = A = 129.9434Kmol/hr.

Feed temperature 120˚C

At the Top of Column

Toluene at top = 1.6371Kmol/hr.

Benzene at top = 2.4557Kmol/hr.

Q_1 = m × latent heat of condensation

Q_1 = 1.6371Kmol/hr×0.03301KJ/Kmol+2.4557×0.02777KJ/Kmol

Q_1 = 0.1221

Outlet temperature is 60˚C for top

$Q_2 = mC_p\Delta T + mC_p\Delta T$

Q_2 = 1.6371×157.2(383.6-333) +2.4557×31.35(353-333)

Q_2 = 14561.7403KJ/hr.

Bottom Product:

Molar Flow rate of Bottom Product = 125.8627Kmol/hr.

C_p Ethylbenzene = 185.372KJ/Kmol

C_p Styrene = 183.2KJ/Kmol

$Q=mC_p\Delta T + mC_p\Delta T$

Q = 44.0520Kmol/hr.×185.372KJ/Kmol (403-393) +81.8107×183.2KJ/Kmol (403-393)

Q = 231537.2754KJ/hr.

4.6 Distillation Column 2 (T-101)

Ethylbenzene at the top = 43.1882Kmol/hr.

Q_1 = m×Latent heat of condensation

Q_1= 43.1882Kmol/hr.×0.40934KJ/Kmol

Q_1= 17.6787KJ/hr.

Outlet temperature is 130˚C

$Q_2 = mC_p\Delta T$

Q_2 = 43.1882Kmol/hr.×185.372KJ/Kmol(409K-403K)

Q_2= 48035.2981KJ/hr.

Styrene at the Bottom = 80.2066Kmol/hr.

$Q = mC_p\Delta T$

C_p = 183.2KJ/Kmol

Q= 80.2066Kmol/hr.×183.2KJ/Kmol(418K-403K)

Q = 132244.6421KJ/hr.

4.7 Bubble Point Calculation of Feed

So, the enthalpy of feed at its bubble point is

$$\Delta H_{fs} = 16311.\frac{3KJ}{kmol}$$

And latent heat of feed at 338K is,

$$\Delta H_f = \frac{5162.87KJ}{kmol}$$

And latent heat of feed at 338K is,

Λ=46389.61KJ/kmol

So,

q=1.24

As the value of q is greater than 1 so,

Condition of feed: Cold Liquid

4.7.1 Top Temperature

As the column pressure at the top is 740 mmHg so, at this pressure using Antoine equation the temperature is 460.5K, which is calculated as under,

TABLE 4-2 VALUES UNDER GIVEN PRESSURE AND TEMPERATURE

Pressure = 740 mm Hg

Temperature = 406.5 K

	Vapor Pressure	K-value	Xd	Xd/K

Ethyl Benzene (Lk)	718.0252	0.9703	0.92	0.9481
Styrene (HK)	549.3775	0.7424	0.02	0.0269
Toluene	1390.5604	1.87913	0.04	0.0212
Benzene	3061.8271	4.2376	0.02	0.0048
			1	1.0012

4.8 Dew Point Calculation at Top

And the vapor flow rate at the top of the column is 326.39 kmol/hr.

So, at this temperature the enthalpy of vapor is,

$$\Delta Hvap = \int CpdT = 83.78 \times \int Cp\, dT$$

As

$$Cp\Delta T = -41.867 + 0.6914T - 0.00047T^2$$

So,

$$\Delta H_{vap} = 326.39 \int_{298}^{406.6} (-41.867 + 0.6914T - 0.00047T^2)dT$$

$$\Delta H_{vap} = 326.39 \times (-41.867 \times (406.6 - 298) + 0.6914(406.6^2 - 298^2) - 0.00047(406.6^3 - 298^3))$$

$$\Delta H_{vap} = 326.39 \times (-4542.6 + 26434.7 - 637.75)$$

$$\Delta H_{vap} = 326.39 \times (21244.35)$$

ΔH_{vap} = 6933943.4 KJ/hr.

4.9 Bottom Temperature

And at the bottom of the column the pressure is 760 mmHg and the temperature is estimated as,

TABLE 4-3 VALUES UNDER GIVEN PRESSURE AND TEMPERATURE

Pressure = 760 mmHg

Temperature = 418.2K

	Vapor pressure	K-value	Xd	Xd × K
Ethyl Benzene (LK)	977.4051	1.28659	0.02	0.02572
Styrene (HK)	756.9461	0.9959	0.98	0.9760
			1	1.0017

4.10 Bubble Point Calculation at Bottom

Now the enthalpy of the bottom product is,

$\Delta H_L = 56.12 \times \int_{298}^{418.2} (-28.54 + 0.617T - 0.00041T^2)\, dT$

$\Delta H_L = 56.12 \times \int_{298}^{418.2} (-28.54 \times (418.2 - 298) + \frac{0.617}{2} (418.2^2 - 298^2) - 0.00041(418.2^3 - 298^2)$

$\Delta H_L = 56.12 \times (-3430.51 + 26557.9 - 6379.04)$

$\Delta H_L = 56.12 \times (16748.35)$

ΔH_L = 939917.4 KJ/hr.

CHAPTER 5

PLANT DESIGN

5 Plant Design

5.1 Reactor Design

5.1.1 Design Equation:

$$F_{Ao}\frac{dX}{dW} = -r_A$$

Integrating the above equation:

$$W=F_{Ao}\int_0^X \frac{dX}{-r_A}$$

Rate Law:

$$-r_A = K_r\left[P_E - \frac{(P_S P_H)^2}{K_e}\right] \text{ (Kgmol/h-Kg catalyst)}$$

Were,

$K_r = exp\left[9.44 - \frac{11000}{T}\right]$

&

$K_r = exp\left[9.44 - \frac{15000}{T}\right]$

In this pressure is in bar and temperature is K.

Stoichiometry:

Gas phase reaction with pressure drop.

Following are the partial pressure of each component multiplied by their mole fraction.

P_{EB}=y_{EB}xP_T

P_S=y_SxP_T

P_H=y_HxP_T

The number of moles changes in reaction 1, the number of moles of ethyl benzene, styrene and hydrogen are (1+X), where X is the conversion rate at any point.

Thus, the mole fraction of reacting species will be.

y_{EB}=(1-X)/(9+X)

y_S=X/(9+X)

y_H=X/(9+X)

So,

P_{EB}=((1-X)/(9+X) xP_T

P_s=((X)/(9+X) xP_T

P_H=((X)/(9+X) xP_T

Combining yields:

$$-r_A = K_r\left[P_T\frac{(1-X)}{9+X} - P_T^2\frac{X^2}{(9+X)^2K_e}\right]$$

Where P_T equals to 120KPa i.e 1.2bar

So,

$$-r_A = K_r\left[1.2\frac{(1-X)}{9+X} - 1.2^2\frac{X^2}{(9+X)^2K_e}\right]$$

$$-r_A = 1.2K_r\left[1.2\frac{(1-X)}{9+X} - 1.2^2\frac{X^2}{(9+X)^2K_e}\right]$$

Simplifying.

$$-r_A = 1.2K_r\left[\frac{(1-X)(9+X)K_e-1.2X^2}{(9+X)^2K_e}\right]$$

$$-\frac{1}{r_A}=\frac{1}{1.2K_r}\left[\frac{K_e(9-X)^2}{1.2X^2-K_e(1-X)(9-X)}\right]$$

$$W=F_{Ao}\int_0^X\frac{1}{1.2K_r}\left[\frac{K_e(9-X)^2}{1.2X^2-K_e(1-X)(9-X)}\right]$$

5.1.2 Energy Balance:

The general energy balance equation is,

Q-$W_{s-}F_{Ao}[\sum\alpha_i\,\theta_i(T-T_O)+\sum\beta_i\ \theta_i(T^2$-$T_o{}^2)\frac{1}{2}+\sum Y_i\theta_i(T^3-T_o{}^3)$/3] –$F_{Ao}X[\Delta H_R{}^o(T_R)+$

$\frac{\Delta\beta(T^2-T_R{}^2)}{2}+\frac{\Delta y(T^3-T_R{}^3)}{3}=0$

Were,

T_R=Reference temperature = 298K

T= Exit temperature of reactor

T_o=Entering temperature of reactor = 873K

$$X= \frac{136.96\ (T-873)+0.3609\ (T^2-873^2)-1.415\times10^{-4}(T^3-873^3)}{117090+49-994(T-298)-0.041(T^2-298^2)+0.0000217(T^3-298^3)}$$

T(K)	**X**
873	0
863	0.034848
853	0.069811
843	0.104882
833	0.140052
823	0.175312
813	0.210655
803	0.246071
793	0.281554
783	0.317094
773	0.352684
763	0.388316

TABLE 5-1

$$W=F_{Ao}\int_0^{0.34}\frac{1}{1.2K_r}\left[\frac{K_e(9-X)^2}{1.2X^2-K_e(1-X)(9-X)}\right]$$

Now to solve the above integral Simpson 1/3 rule is applied as fellow.

X	**T**	$\boldsymbol{K_r}$	$\boldsymbol{K_e}$	$\boldsymbol{-r_A}$	$\boldsymbol{1/{-r_A}}$
0	873	0.042416	0.224893	0.005655	176.82=f_1
0.038	862	0.036116	0.180614	0.004606	217.1074=f_2
0.076	851	0.030624	0.144233	0.003716	269.1248=f_3
0.114	840	0.025855	0.114504	0.002959	337.9835=f_4
0.152	830	0.022082	0.092339	0.002366	422.6028=f_5
0.19	818	0.01818	0.070835	0.001752	570.6736=f_6

0.228	803	0.014142	0.05029	0.001097	911.6324=f_7
0.266	796	0.012537	0.042672	0.000822	1216.719=f_8
0.304	787	0.010704	0.034399	0.000488	2050.821=f_9
0.34	776	0.00878	0.026255	9.67x10^{-5}	10340.52=f_{10}

TABLE 5-2

To evaluate Simpson's 1/3 rule

I=Δh/3 x(f_1+4$(f_2 + f_4 + f_6 + f_8) + 2(f_3 + f_5 + f_7 + f_9) + f_{10})$

Where we have,

Δh=0.038

$f_2 + f_4 + f_6 + f_8$=217.1074+337.9835+570.6736+1216.719

=2342.48

4x$(f_2 + f_4 + f_6 + f_8)$=4x2342.48

=9369.992

$f_3 + f_5 + f_7 + f_9$=3654.18

2x$f_3 + f_5 + f_7 + f_9$=2x3654.18

=7308.36

So,

I=344.48(h-Kg catalyst/Kgmol)

So,

W=$F_{Ao} \times I$

W=83.83x344.48

W=28877.7kg

W≈29000Kg

W≈29 ton

Now bulk density of the catalyst is,

$$\rho_{bulk} = 1440Kg/m^3$$

So,

Bulk volume of the Catalyst bed, =V_B=$\frac{W}{\rho_{bulk}}$=$\frac{29000}{1440}$

V_B=20.13m^3

Now for an adiabatic reactor L/D i.e. length to diameter ratio is 3

So,

Length of the bed = 5x Diameter of the bed

L=3xD

The volume of the catalyst bed is

V_B=LxA

A is the cross-sectional area of the vessel in which catalyst is placed

So,

V_B=$L \times \frac{\pi D^2}{4}$

V_B=$3D \times \frac{\pi D^2}{4}$

V_B=$\frac{3\pi D^3}{4}$

D^3=$\frac{4\times 20.13}{3\pi}$

D^3=8.54m^3

D=2.04m or 6.7ft

So,

A=$\frac{\pi D^2}{4}$

A=$\frac{\pi(2.04)^2}{4}$

A=3.3m^2

A=35.5ft^2

So, length of the bed is,

L=3xD

L=3x2.04

L=6.12m or 20ft

Pressure drop:

To find the pressure drop around the catalyst bed we will use Ergun's Equation i.e.

$$\frac{\Delta P}{L}=\frac{1-\varepsilon}{\varepsilon^3}\times\frac{G^2}{d_p g_c \rho_G}\times\left[\frac{150\times(1-\varepsilon)\mu_G}{d_p G}+1.75\right]$$

From the properties of catalyst:

ε=0.445

d_p=0.0047m or 0.015ft

G=38196.48lb/hr.

G=1075.96lb/hr.-ft^2

L=20ft

μ_G=0.075lb/ft-hr

So,

$\frac{\Delta P}{L}$=18.21lb_f/in^2

=0.91psi/ft

ΔP=0.91xL

ΔP=0.91X20

ΔP=18.2psi or 125.4KPa

5.2 Distillation Column:

5.2.1 Flow Rate:

The condition of the Distillation column as described in energy balance is at its cold liquor so,

q=1.24

By using Underwood's equation, the minimum reflux ratio is as follows,

$$\frac{\alpha_A \times \alpha_{fA}}{\alpha_A - \theta} - \frac{\alpha_B \times \alpha_{fB}}{\alpha_B - \theta} + \frac{\alpha_C \times \alpha_{fC}}{\alpha_C - \theta} = 1 - q$$

$$\frac{1.3 \times 0.317}{1.3 - \theta} - \frac{1 \times 0.663}{1 - \theta} + \frac{2.48 \times 0.013}{2.48 - \theta} + \frac{5.39 \times 0.007}{5.39 - \theta} = 1 - 1.24$$

q=-0.24

The value of θ exists betwwen the volatility of light and heavy key, so,

1.3≥ θ ≥1

By solving this by using hit and trail method.

At $\theta = 1.1795,$ so we get above equation at -0.24

So, calculating minimum reflux ratio

$$\frac{\alpha_A \times \alpha_{fA}}{\alpha_A - \theta} - \frac{\alpha_B \times \alpha_{fB}}{\alpha_B - \theta} + \frac{\alpha_C \times \alpha_{fC}}{\alpha_C - \theta} = R_m + 1$$

$$\frac{1.3 \times 0.317}{1.3 - 1.1795} - \frac{1 \times 0.663}{1 - 1.1795} + \frac{2.48 \times 0.013}{2.48 - 1.1795} + \frac{5.39 \times 0.007}{5.39 - 1.1795} = R_m + 1$$

R_m =9

Now,

Operating on a reflux ratio of 1.2-1.25

R=1.2+9

=10.8

$\frac{R_m}{R_m+1}$=0.9

$\frac{R}{R+1}$=0.091

We came to know from the graph Erbar Maddox that,

${N_m}/{N}$=0.5

Where we have,

R=Operating Reflux ratio

R_m= minimum Reflux ratio

N= Number of stages operating at R

N_m= Minimum number of stages obtained by Fenske method

Minimum Number of plates:

By applying Fenske's Equation, we can find the number of plates for desired separation under condition of total reflux.

N_m+1=$\frac{\log\left[({}^{X_A}/_{X_B})_D({}^{X_B}/_{X_A})_B\right]}{\log(\alpha_{AB})_{av}}$

N_m+1=$\frac{\log[({}^{0.92}/_{0.02})({}^{0.98}/_{0.02})]}{\log 1.3}$

so, by solving we get,

N_m=29.4≈29 trays

From this we get the theoretical number of plates=N=29/0.5=58 trays

One of these plates account for the reboiler that's why we have 57 plates.

Using O'Connell's method, we get,

Plate efficiency=69%=0.69

Actual number of plates=57/0.69=82 plates

For calculating the number of plats above and below the feed plate, by using the formula.

$$\log {}^{N_e}/_{N_s} = 0.206 \log\left[(X_H/X_L)_F\,(\frac{W}{D})(X_{L,W}/X_{H,D})^2\right]$$

$$\log {}^{N_e}/_{N_s} = 0.206 \log\left[(\frac{0.663}{0.317})(\frac{56.12}{27.65})(0.02/0.02)^2\right]$$

$$\log {}^{N_e}/_{N_s} = 0.206 \log(4.245)$$

${}^{N_e}/_{N_s}$=1.347

As we know now,

N=$N_e + N_s$

82=$N_e + N_s$

Now we have,

N_e=23

N_s=25

Feed= 83.78Kmol/hr.

As mass balance on ethylbenzene gives:

Top product D=27.66Kmol/hr.

Vapor Rate =Dx(1+R) =27.66x(1+10.8)

=326.39Kmol/hr.

An overall mass balance Gives;

Bottom Product

B=83.78-27.66=56.12Kmol/hr.

Vapor rate =V_m'=L_m'-B

Foer which we have, \

Vapor flow rate below feed = 346.5kmol/hr.

Liquid flow rate below feed = 402.62kmol/hr.

Physical Properties:

TABLE 5-3 PHYSICAL PROPERTIES

Properties	Top	Bottom
Liquid Rate (kmol/hr.) or (lbmol/hr.)	298.73(658)	402.62(886.83)
Vapor-Rate(kmol/hr.) or(lbmol/hr.)	326.39(718.9)	346.5(763.21)
Vapor Molecular weight	105	104.2
Temperature K	406.6	418.2
Pressure mmHg	740	760

Liquid Density Kg/m^3or lb/ft^3	754.95(47.1)	789.24(49.2)
Vapor density Kg/m^3or lb/ft^3	3.06(0.19)	3.03(0.189)
Liquid surface tension	16.92	18.246

Column Diameter:

Assumed tray spacing =20in=0.5m

Turn down ratio=0.7

Maximum Vapor Velocity.

Top

$$\frac{L}{G}\left[\frac{\rho_G}{\rho_L}\right]^{0.5}$$

$$\frac{L}{G}\left[\frac{\rho_G}{\rho_L}\right]^{0.5}=\frac{658}{718.9}\left[\frac{0.19}{47.1}\right]^{0.5}$$

=0.06

We have from appendix A table A1.

K_v'=0.32

$$V_m=K_v'\left[\frac{\sigma}{20}\right]^{0.2}\left[\frac{\rho_L-\rho_G}{\rho_L}\right]^{0.5}$$

$$V_m=K_v'\left[\frac{\sigma}{20}\right]^{0.2}\left[\frac{\rho_L-\rho_G}{\rho_L}\right]^{0.5}$$

$$V_m=0.32\left[\frac{16.92}{20}\right]^{0.2}\left[\frac{47.1-0.19}{0.19}\right]^{0.5}$$

V_m=4.86ft/s

Let the operating velocity be the 80% of maximum velocity in the tower, so,

Operating Velocity=V=0.8V_m

=0.8x4.86

=3.888ft/s

Diameter.

$$D=\left[\frac{4\times G\times M}{\pi\times\rho_G\times V}\right]^{0.5}$$

$$D=\left[\frac{4\times 718.9\times 105}{\pi\times 0.19\times 3.888\times 3600}\right]^{0.5}$$

D=6ft

Bottom:

$$=\frac{L}{G}\left[\frac{\rho_G}{\rho_L}\right]^{0.5}$$

$$=\frac{886.82}{718}\left[\frac{0.189}{49.2}\right]^{0.5}$$

=0.072

From appendix A table A1;

K_V'=0.31

$$V_m=K_V'\left[\frac{\sigma}{20}\right]^{0.2}\left[\frac{\rho_L-\rho_G}{\rho_G}\right]^{0.5}$$

$$=0.31\left[\frac{18.246}{20}\right]^{0.2}\left[\frac{49.2-0.189}{0.189}\right]^{0.5}$$

=4.9ft/s

Operating velocity is 80%so,

Operating velocity=0.8V_m

=0.8 x4.9ft/s

=3.92ft/s

Diameter:

$$D=\left[\frac{4\times G\times M}{\pi\times\rho_G\times V}\right]^{0.5}$$

$$D=\left[\frac{4\times 763.21\times 104.2}{\pi\times 0.189\times 3.92\times 3600}\right]^{0.5}$$

D=6.2ft

Cross-sectional area of the tower;

$A_C = \frac{\pi D^2}{4}$

$= \frac{\pi (6.2)^2}{4}$

$=30.2 ft^2$

Liquid Flow arrangement:

Top:

At the top of the tower;

$L = \frac{298.73 kmol}{hr} \times \frac{1 ht}{3600 s} \times \frac{105 Kg}{1 kmol} \times \frac{m^3}{754.95 kg}$

L=1.15 x $10^{-2} m^3/s$

From table A2 from appendix A;

Liquid flow arrangement= Cross Flow (Single Pass)

$L = \frac{402.62 kmol}{hr} \times \frac{1 ht}{3600 s} \times \frac{105 Kg}{1 kmol} \times \frac{m^3}{754.95 kg}$

L=1.47x $10^{-2} m^3/s$

Plate Design:

Sieve hole diameter=$d_\circ = 4.5 mm$=0.015ft

Weir Length=l_w= 0.7xD

=0.7x6.2

=4.34ft

Weir height=h_w=50mm=0.16ft

Down comer skirt height= Weir height-10mm

=50-10

=40mm

=0.13ft

From table A3 in appendix A;

For weir length=0.7xD

Distance from center of tower=0.3562x D

=0.3562x6.2

=2.21ft

=0.67m

Tower area used by one downspout=8.81%x D

=8.81%x30.2

=2.66ft^2

=2.7ft^2

For hole diameter=4.5mm=3/16 in

From table A4 in appendix A;

$\frac{Plate\ thickness}{Hole\ Diameter}$=0.43

And typical active area =$\frac{A_a}{A_c}$=0.74

A_a=0.74xA_c

A_a=0.74x30.2

A_a=22.35ft^3

A_a=2.07m^2

Triangular pitch layout;

P'=12mm=0.04ft

$\frac{A_o}{A_a}$=0.907$\left[\frac{d_o}{p}\right]^2$

$\frac{A_o}{A_a}$=0.907$\left[\frac{0.015}{0.04}\right]^2$

$\frac{A_o}{A_a}$=001275

So,

Summarizing all the area and length we have,

Column Diameter= D=6.2ft

Column Area=A_C=30.2ft^2

Down comer Area=A_d=2.7ft^2

Net area =A_n=A_c−A_d=30.2-2.7=27.5ft^2

Active area =A_a=A_c−$2A_d$=22.35ft^2

Hole area $A_h$take 10%A_a as first trail=2.235ft^2

Sieve hole diameter=d_o=4.5mm=0.015ft

Weir length =l_W=4.3ft

Weir height=h_W=0.16ft

5.3 Separator Design:

Separator Data Required:

Liquid Flow Rate= W_L= 578.43Kmol/hr=10.7lb/s

Vapor Flow Rate= W_V= 81.6Kmol/hr.= 1.04lb/s

Density of Liquid = ρ_L =756.07Kg/m^3= 47.15lb/ft^3

Density of vapor=ρ_V=0.55Kg/m^3=0.034lb/ft^3

Separation Factor:

$$\frac{W_L}{W_V}\left[\frac{\rho_V}{\rho_L}\right]^{0.5} = \frac{10.7}{1.04}\left[\frac{0.034}{47.15}\right]^{0.5} = 0.276$$

Form Appendix A, we Have,

K_V=0.37

And,

K_H=1.25K_V

$K_H = 1.25$ x 0.37

K_H=0.4625

Maximum Velocity:

$$U_{vapor\ max} = K_H \left[\frac{\rho_L - \rho_V}{\rho_V}\right]^{0.5}$$

$U_{vapor\ max}$ = 0.4625$\left[\frac{47.15-0.034}{0.034}\right]^{0.5}$

$U_{vapor\ max}$= 17.2ft/s

Operating Velocity=U=85%$U_{vapor\ max}$

U=0.85 x $U_{vapor\ max}$

U=0.85 x 17.2ft/s

U= 14.62ft/s

Required vapor Flow Area:

A_V=$\frac{Q_V}{U}$=$\frac{30.6}{14.62}$

A_V=2.09ft^2

Design Surge Time is

t = 10min

so,

Full liquid Volume = Q_L x t

V=0.23 x 10 x 60

V = 138ft^3

Total Area = $A_T = \frac{A_V}{0.2}$

=$\frac{2.09}{0.2}$

= 10.45ft^2

And,

Diameter = D = $\left[\frac{4 \times A_T}{\pi}\right]^{0.5}$

D=$\left[\frac{4\times 10.45}{\pi}\right]^{0.5}$

D= 3.64ft

D_{Actual}= D to next largest six inches 6"

D_{Actual}=3.63 to next largest six inches 6"

D_{Actual}=4ft

Vessel Length:

L= $\frac{Full\ Liquid\ Volume}{\frac{\pi D_A^2}{4}}$

L=$\frac{138}{12.56}$

L=10.98ft

${}^{L}/_{D}$=3.0

5.4 Kettle Reboiler:

Thermal Design:

Only the thermal design and general layout will be done

Mass Flow=56.12kgmol/hr.

=56.12 x 104.2

=$\frac{5847.7}{3600}$

=1.624kg/s

Physical Properties of mixture at 760mmHg

Boiling Point= 418.2K

=145.05℃

Latent Heat= 401kJ/kg

Mean Specific Heat= 1.38KJ/Kg

Critical Pressure= 39.82bar

Heat Load:

Sensible heat (maximum) = $C_p \Delta T$

= 1.38 x (145.05 -25)

= 165.67KJ/Kg

Total heat load= (Sensible heat + Latent Heat) x Mass Flow

= (165.67 +401) x 1.624

=566.67 x 1.624

=920.5KJ/s

=920.5KW

Adding 5% heat loss;

Maximum Heat load (Duty) =1.05 x 920.5

=966.52KW

Assume overall heat transfer Coefficient;

$$U_\circ = 1000 \, {}^{W}\!/_{m^2 {}^\circ\mathrm{C}}$$

Mean Temperature Difference; both sides isothermal,

Steam saturation temperature at 15.5 bar = 200℃

$$\Delta T_m = 200 - 145.5$$

=54.95℃

Area (outside) required = A= $\frac{Q}{U_\circ \Delta T_m}$

= $\frac{966.52 \times 10^3}{1000 \times 54.95}$

=17.6m^2

Select,

Internal diameter = 25mm

Outer diameter = 30mm

Nominal length = L = 4.8m (one U-tube)

Number of U-tubes = $\frac{A}{OD\times\pi\times L}$

=$\frac{17.6}{30\times10^{-3}\times\pi\times4.8}$

=39 tubes

Pitch arrangement:

Pitch = 1.5 x OD

=1.5 x 30

=45mm

This given layout gives 40 U-tubes.

Bundle Diameter;

$$D_B = d_\circ \left[\frac{N_t}{K_1}\right]^{1/n_1}$$

We have;

$$K_1 = 0.156$$

$$n_1 = 2.091$$

So,

$$D_b = 30 \times \left[\frac{80}{0.156}\right]^{1/2.291}$$

$$D_b = 457\ mm$$

Boiling Co-efficient:

By using Mostinski equation:

Heat Flux Based on estimated area,

q=$\frac{Q}{A}$

=$\frac{966.52}{17.6}$

=54.9KW/m^2

$$h_{n,b} = 0.104 \times (P_c)^{0.69} \times (q)^{0.7} 1.8 \left[\frac{P}{P_c}\right]^{0.17} + 4\left[\frac{P}{P_c}\right]^{1.2} + 10\left[\frac{P}{P_c}\right]^{10}$$

$$h_{n,b} = 0.104 \times (39.82)^{0.69} \times (54.9 \times 10^3)^{0.7} (1.8\left[\frac{1}{39.82}\right]^{0.17} + 4\left[\frac{1}{39.82}\right]^{1.2} + 10\left[\frac{1}{39.82}\right]^{10})$$

$$h_{n,b} = 0.104 \times (12.71) \times (2078.26) \times [1.8(0.534) + 4(0.012) + 10(9.97 \times 10^{16})]$$

$$h_{n,b} = 0.104 \times 12.71 \times 2078.26 \times 1.0092$$

$$h_{n,b} = 2722.4 W/m^2 °\mathrm{C}$$

Take,

Steam Condensation Co-efficient= 8000 $W/m^2 °\mathrm{C}$

Steam Fouling Co-efficient = 5000 $W/m^2 °\mathrm{C}$

Mixture Fouling Co-efficient = 10000 $W/m^2 °\mathrm{C}$

Tube Material will be plain carbon steel,

So,

$$K_W = 55 W/m^2 °\mathrm{C}$$

So,

$$\frac{1}{U_\circ} = \frac{1}{h_O} + \frac{1}{h_{O,d}} + \frac{OD \times \ln(OD/ID)}{2 \times K_W} + \frac{OD}{ID} + \frac{1}{h_i} + \frac{1}{h_{i,d}}$$

$$\frac{1}{U_\circ} = \frac{1}{2722.4} + \frac{1}{10000} + \frac{30 \times 10^{-3} \ln(30/25)}{2 \times K_W} + \frac{30}{25} + \frac{1}{5000} + \frac{1}{8000}$$

$$\frac{1}{U_\circ} = 0.00047 + 0.00005 + 0.00039$$

$$\frac{1}{U_\circ} = 0.00091$$

$$U_o = \frac{1}{0.00091}$$

$$U_o = 1098.9\,{}^{W}\!/_{m^2{}^\circ\mathrm{C}}$$

Maximum allowable Heat Flux:

Using Modified Zuber Equation

Surface Tension = $\sigma = 18.246 mN/m$

=18.26$\times 10^{-3}$

Density=ρ_L =789.24Kg/m^3

Density=ρ_G=3.03kg/m^3

No. of tubes = N_t=2$\times U - tubes$=2x40

=80

For square arrangement;

$$K_b = 0.44$$

So,

$$q_c = K_b \times \frac{P_t}{OD} \times \frac{\lambda}{\sqrt{N_t}} \times [\sigma \times g(\rho_L - \rho_V) \times \rho_V^2]^{0.25}$$

$$q_c = 0.44 \times 1.5 \times \frac{401 \times 10^3}{\sqrt{80}} \times [18.246 \times 10^{-3} \times 9.81(789.24 - 3.03) \times 3.03]^{0.25}$$

$$q_c = 1777388.43\,{}^{W}\!/_{m^2}$$

$$q_c = 177.4\,{}^{KW}\!/_{m^2}$$

Applying the factor of 0.7,

Maximum Flux Limit=$q_C' = 0.7 \times q_c$

=0.7$\times$ 177.4

=124.18${}^{KW}\!/_{m^2}$

The calculated value of the flux is =q=54.9${}^{KW}\!/_{m^2}$

Is well below maximum allowable.

Layout:

From Tube sheet layout;

D_b=457mm

By taking shell diameter as twice bundle diameter

D_S=D_bx2

=2x457mm

=914mm

Take liquid level as 500mm from base,

Freeboard= 914-500

=414mm, satisfactory

CHAPTER 06

PROCESS INSTRUMENTATION

6 Instrumentation:

6.1 Introduction:

To monitor the key process variables during plant operations instrumentation is used. Instruments can be automated control loops or manually operated ones to monitor the process operations. These instruments are generally connected to a computer automated data gathering system. These instruments which are monitoring critical process variables will be fitted with automatic alarms to alert the operators about critical and hazardous situation.

6.2 Instrumentation and control Objectives:

The key objectives while designing is to specify these instrumentation and control schemes as following.

Safe Plant Operations:

a) To keep the process variables within the known parameters of safe operating limits.

b) To detect dangerous situation as they develop and to provide alarms that automatically shut down the systems

Production rate:

To achieve the maximum designed product output.

Product Quality:

To maintain the product composition within the specific quality standards.

Cost:

To operate at the lowest production cost at which the plant is designed.

6.3 Components of the Control Systems:

6.3.1 Means of measurement:

The most important element in a control system are the means of the measurements. If measurements are not calculated properly the rest of the system cannot operate optimally.

Variables to be measured:

a) Pressure Measurement:
b) Temperature Measurements
c) Flow rate Measurements.
d) Level Measurements.

Variables to be Recorded

a) Indicated Temperature
b) Composition.
c) Pressure.

6.3.2 Controller:

The mechanism that calculate and detect the error is called controller. The controller consists of an error-detecting mechanism which compares the measured variables with the desired values of the measured variables, this difference is called error.

6.3.2.1 Final Control Element:

The final control element gathers data from the controller in the forms of signals and by some predetermined levels changes the energy input to the process.

6.3.2.2 Classification of Controllers:

Commonly, the process controllers are classified as:

a) Pneumatic Controllers.
b) Electronic Controllers
c) Hydraulic Controllers.

6.3.2.3 Modes of Controllers:

Modes refers to the different ways or methods used to manage or regulate a system, process, or activity. These modes can include various tools, techniques, and strategies that are employed to ensure that the desired outcomes are achieved and that the system remains within specified parameters or limits. Examples of modes of control include feedback loops, sensors, automation, manual intervention, and various monitoring and analysis tools. The four basic modes of controls are as following.

1. On-Off Control
2. Integral Control
3. Proportional Control
4. Rate or Derivative Control

In industry integral, proportional or derivative modes seldomly occurs alone in the control system.

6.3.3 Alarms Safety trips and interlocks:

Alarms are used to alert the operators of any serious and potentially hazardous deviations which occur I the process condition. The significant instruments are fitted with switches and relays to operate audible and visual alarms on the control panels.

The basic components of Automatic trip systems are:

1. A sensor to monitor the control variable and provide an output signal when a preset is exceeded.
2. A link to transfer the signal to the actuator usually consisting of a system of pneumatic or electric relays.
3. An actuator to carry out the required action, close or open a valve, switch off a motor.

6.3.3.1 Interlocks:

Interlocks are important safety devices that prevent unsafe events in systems or processes by halting specific actions until conditions are met. These mechanisms can be mechanical, electrical, or electronic and are used in complex systems such as industrial machinery, chemical plants, and nuclear reactors. Interlocks are critical in preventing errors or malfunctions that could have severe consequences.

6.3.3.2 Flow Controller:

A flow controller is an essential instrument that regulates the flow of fluids or gases in a process control system by comparing actual and desired flow rates and adjusting a control valve. It is crucial for various industries, including chemical processing, food and beverage production, pharmaceutical manufacturing, and wastewater treatment. Flow controllers can be operated manually, automatically, or through a computerized system, ensuring system efficiency and reliability.

6.3.3.3 Temperature Controller:

A temperature controller is an instrument that regulates and maintains a desired temperature in a system. It receives temperature information through a sensor and compares it to the desired setpoint. It can adjust a heating or cooling device based on the comparison to achieve the desired temperature.

6.3.3.4 Pressure Controller:

A pressure controller is an instrument used in process control to regulate and maintain a desired pressure within a system. It receives information about the pressure through a pressure sensor and compares it to the desired pressure setpoint. Based on this comparison, the pressure controller can adjust a control device, such as a valve or pump, to achieve and maintain the desired pressure.

6.3.3.5 Level Controller:

A level controller is an important instrument in process control that regulates and maintains a desired level of liquid or solid material within a system. It compares the actual level to the desired level using a level sensor and adjusts a control device, such as a valve or pump, to achieve and maintain the desired level.

6.3.3.6 Control Valve:

A control valve is a critical component in instrumentation and process control systems that is used to control the flow, pressure, temperature, or level of a fluid or gas in a process. It is an automatic valve that can be adjusted to regulate the flow of fluid or gas to maintain a desired process parameter. Control valves are used in a wide range of industries, including chemical processing, oil and gas, power generation, and wastewater treatment. They can be operated manually or automatically through a control signal from a process controller.

6.4 Control System for Equipment:

6.4.1 Ratio Control Loop on Mixing Point (M-100)

Our objective is to keep the ratio of the fresh Ethyl Benzene Feed to the Steam at a specified value. To fulfil this purpose, we will use a Divider a flow transmitter and a control valve.

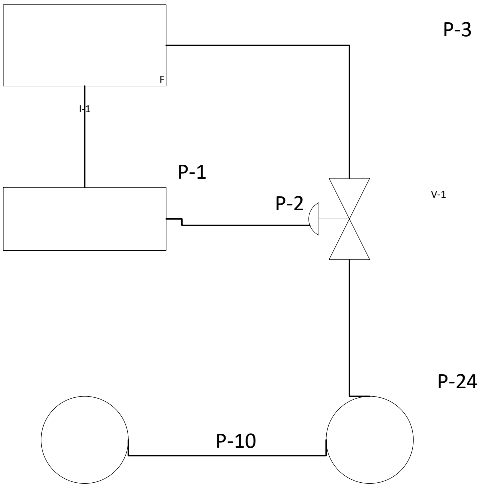

FIGURE 6-1

6.4.2 Feed-Back Control Loop on Reactor (R-100, R-101)

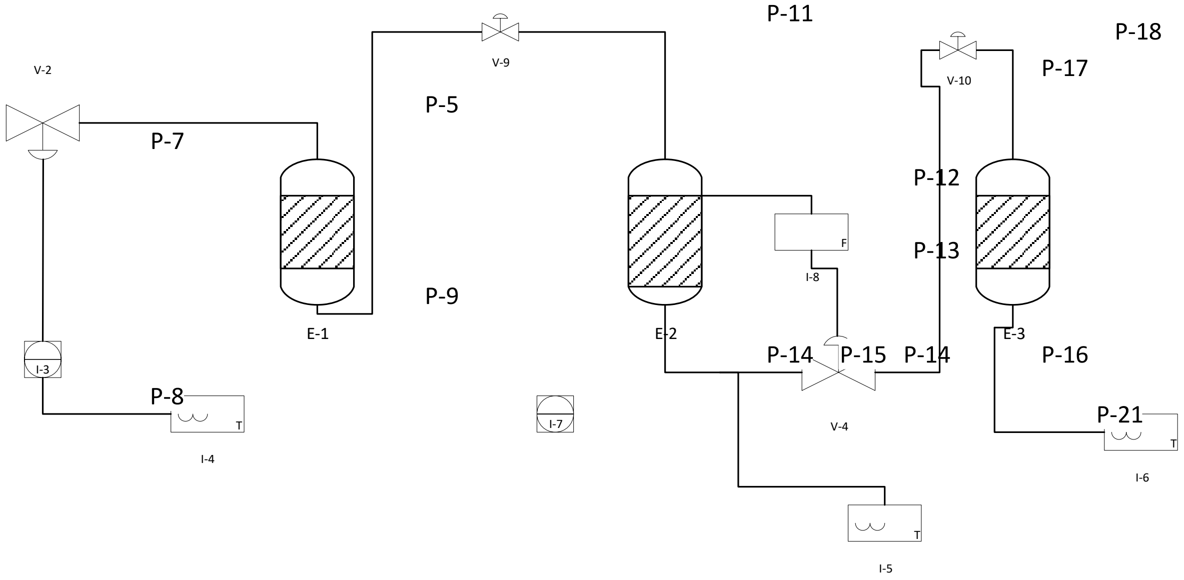

FIGURE 2 IPC ON REACTORS

TABLE 6-1 TOTAL QUANTITIES

Total Number of Variables (Excluding Constant Parameters)	9	[V, Fi, Ti, cAi, pi, F_0, T_0, cA_0, p_0]
Externally Specified	4	[F_i, Ti, cAi, pi, F_0, or T_0]
Unspecified Variables	5	
Number of Modeling Equations	4	Mass Balance Heat Balance Component A Balance Component B Balance
Number of manipulated and Controlled Variables	1	

6.4.3 Feed Bed Control on Loop on Distillation Column:

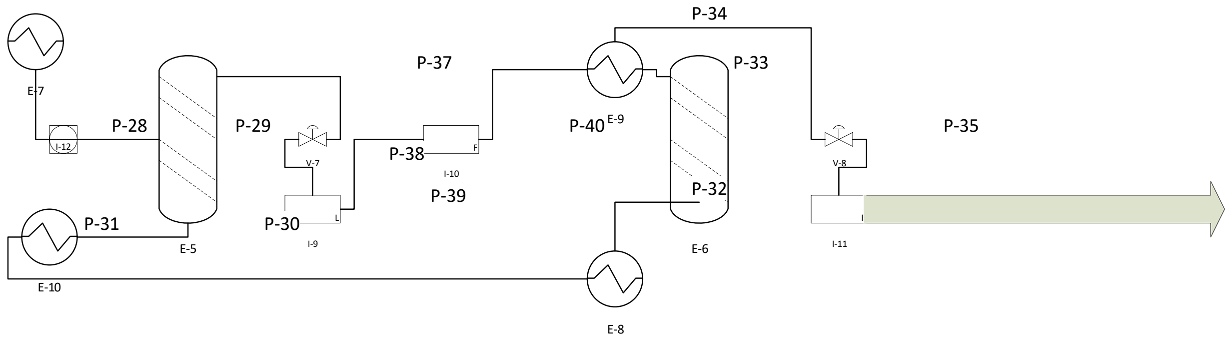

FIGURE 3 IPC ON DISTILLATION

TABLE 6-2 IPC VALUES

Total Number of Variables	N+2	Liquid Vapor Pressure
(Excluding Constant Parameters)	N+1	Vapor Pressure
	N+2	Liquid holdups
	N	Liquid Flows
	6	F_f, F_D, F_B,F_R,c_f,V
Total	4N+11	
Externally Specified	2	F_f , c_f
Unspecified Variables	4N+9	
Number of modeling Equations	N+1	Equilibrium Relationship
	N	Hydraulic Relationships
	2	Balances around the feed tray
	2	Balances around the top tray
	2	Balances around the bottom
	2(N-3)	tray
	2	Balances around the ith tray;
	2	i≠1, N,f

		Balances around the reflux drum Balances around the Column base
Total	4N+5	
Number of manipulated and controlled Variables	(4N+9) -(4N+5) = 4	

6.5 Process and Instrumentation Diagram

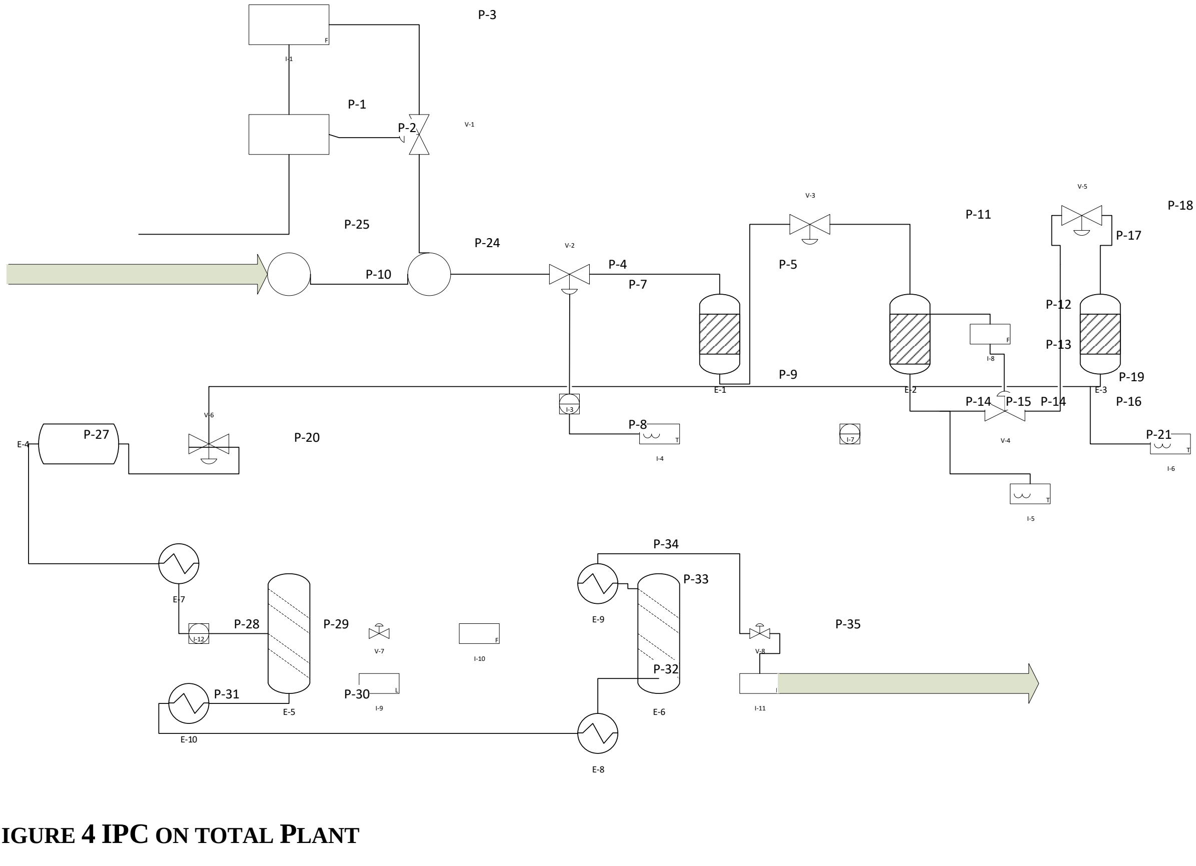

FIGURE 4 IPC ON TOTAL PLANT

Chapter 7

Material of Construction

7 Material of Construction:

Styrene is unsaturated aromatic monomer with a pH ranging between 4-8. It is a solvent which have ability to dissolve many polymeric compounds.

7.1 Types of Materials:

7.1.1 Aluminum Alloys:

The alloys of aluminum are resistant to styrene. They effect the polymerization and help the monomer to remain stable.

7.1.2 Steel and Cast Iron:

Steel and Cast Iron are resistant to the corrosion that is caused by the monomer. These are already being used for shipment of the monomer.

7.1.3 Copper and it’s Alloys:

Styrene is a chromophore compound long exposure to copper effect the stability of the compound.

7.1.4 Nickel Alloys

Nickel and its alloys are resistant to the effects of the monomer but they are not commonly used in the field for styrene because of the stability of stainless steel**.**

7.1.5 Reactive Metals

Most of the reactive metals are resistant to the effects of the monomer but they are not used in the process because of the involvement of other elements.

7.1.6 Precious metals

These types of materials do not find any application in this field.

7.1.7 Other Metals and Alloys

Lead, Zinc and tin are fully resistant, but they are used as trace elements in the Alloys f different metals.

7.1.8 Non-Metallic materials

Non-metallic materials such as polymeric plastic is soluble in the monomer and can form co-polymers so organic non-metallic materials cannot be used. On the other end of the prism we have Glass and Ceramic ware which is not suitable for the job.

7.2 Pitfalls:

If the monomer is stored in a non-reactive container there less chances of a pitfall. On the other hand, the monomer polymerases itself under some conditions

7.3 Material for Equipment Construction:

7.3.1 Material for Reactor (R-100, R-101, R-102)

The material used for the Construction of the Reactors is carbon steel which have high pressure and temperature withstanding ability.

7.3.2 Material for separator(S-100)

The Material for constructing this equipment is Carbon steel.

7.3.3 Material for Distillation Columns (T-100, T-101)

For distillation columns carbon steel is used.

7.3.4 Material for Kettle Re-Boiler:

For Kettle Re-Boiler Carbon Steel will be used.

7.4 Material For storage and Handling:

TABLE 7-1 CONSTRUCTION MATERIAL

Tanks	Steel
Tanks Trucks	Steel
Railroad Carts	Steel
Piping	Steel
Valves	Steel(S41000trim)

Pumps	CF8M or CF8
Gaskets	Spiral-wound PTFE/Stainless steel

CHAPTER 08

COST ESTIMATION

8 Cost Estimation:

8.1 Cost Estimation of Reactor (R-100)

Volume of the Reactor=8.3 m^3

Weight Of the reactor= 879 Kgs

Material of Construction is Carbon steel.

Bare vessel Cost= $84000

Material factor = 1.0

Pressure factor = 1.3

Vessel cost = 84000 x 1x1.3 =109200

Total Cost of the reactor will be= Original Cost x $\frac{\text{Index Value at present}}{\text{Index value at time orignal Cost was obtained}}$

$=\$109200 \times \frac{780.724}{593.7}$

=$143598

8.2 Cost Estimation of Reactor (R-101)

Volume of the Reactor = 10.9 m^3

Weight of the Reactor = 987 Kgs

Material of Construction is Carbon Steel.

Bare Vessel Cost =$ 18000

Material Factor = 1.0

Pressure Factor = 1.3

Vessel Cost = 18000×1.0×1.3 =$23400

Total Cost of the Reactor = $Orignal\ Cost \times \frac{Index\ Value\ at\ present}{Index\ value\ \ at\ time\ orignal\ Cost\ was\ obtained}$

$=\$23400\times\frac{780.724}{593.7}$

=$30771

8.3 Separator Cost (S-100)

Volume of the Separator = 12.3m^3

Weight of the Separator = 1234 Kg

Material of Construction is Carbon steel.

Bare Vessel Cost=$12000

Material Factor = 1.0

Pressure Factor = 1.0

Vessel Cost =$12000 ×1.0×1.0

Total cost of Separator= $Orignal\ Cost \times \frac{Index\ Value\ at\ present}{Index\ value\ \ at\ time\ orignal\ Cost\ was\ obtained}$

=$12000×$\frac{780.724}{593.7}$

=$15780

8.4 Styrene Tower Cost (T-100)

Volume of the vessel = 10.9m^3=$13370.9374

Weight of the vessel= 1356kg

Material of construction is Carbon Steel.

Bare vessel Cost = $180000

Material factor = 1.0

Pressure Factor = 1.0

Vessel Cost = $180000×1×1 =180000

Sieve tray Cost =$960

Total Number of trays = 82

Selectivity factor for 82 trays = $960××0.97 =$76358.4

Total cost of tower=$180000+$76358.4 =$256358.4

Total Cost of Styrene tower= $Orignal\ Cost \times \frac{Index\ Value\ at\ present}{Index\ value\ \ at\ time\ orignal\ Cost\ was\ obtained}$

=\$256358.4×$\frac{780.724}{593.7}$

=\$337111.2960

8.5 Kettle Re-Boiler Cost (K-100)

Bare Cost =\$10800

Type Factor = 1.3

Pressure factor = 1.0

Purchased cost = \$10800×1.3×1.0 =\$14040

Total Cost = $Orignal\ Cost \times \frac{Index\ Value\ at\ present}{Index\ value\ \ at\ time\ orignal\ Cost\ was\ obtained}$

=\$14040×$\frac{780.724}{593.7}$

=\$18462.6

8.6 Distillation Column Cost (T-100)

Volume of the vessel = 9.87m^3

Weight of the vessel= 856kg

Material of construction is Carbon Steel.

Bare vessel Cost = \$22800

Material factor = 1.0

Pressure Factor = 1.0

Vessel Cost = \$22800×1×1 =22800

Sieve tray Cost =\$360

Total Number of trays = 45

Selectivity factor for 45 trays = \$360×45×1.15 =\$18630

Total cost of tower=\$22800+18630 =\$41430

Total Cost of Styrene tower= $Orignal\ Cost \times \frac{Index\ Value\ at\ present}{Index\ value\ \ at\ time\ orignal\ Cost\ was\ obtained}$

=\$41430×$\frac{780.724}{593.7}$

=$54480.45

8.7 Total Purchase Cost:

TABLE 8-1 TOTAL PURCHASE COST

Reactor (R-100)	$143598
Reactor(R-101)	$30771
Separator (S-100)	$15780
Styrene tower (T-100)	$337111.296
Distillation Column	$54480.45
Kettle Re-Boiler	$18462.6
Total Cost	$600203.346

8.8 Total Cost of Plant:

TABLE 8-2 TOTAL COST ESTIMATION

Direct Cost	
Purchased Equipment Delivered	$3785710.5
Purchased Equipment Installation	$1779283.95
Instrumentation and Controls (installed)	$1362855.9
Piping (Installed)	$2574283.2
Electrical System (Installed)	$416428.2
Building (including Services)	$636427.89
Yard improvements	$378571.05
Services Facilities (Installed)	$2649997.5
Total Direct plant Cost	$13583558.19
Indirect Costs	

Engineering and Supervision	$1249284.6
Construction Expenses	$1552141.35
Legal Expenses	$151428.45
Contractor’s fee	$832856.4
Contingency	$1665712.65
Total Indirect Cost	$5451423.450
Fixed Capital Investment	$19079980.95
Working Capital Investment (15% of total)	$3369282.345
Total Capital Investment	$22449262.85

CHAPTER 09

ECOLOGICAL REPORT

9 Ecological Viewpoints

9.1 General

Tirelessness of styrene in the climate is extremely restricted due to its unpredictability from soils and surface waters, its quick obliteration in air and its biodegradation in soils, and surface and groundwaters.

9.2 Parceling to the Air Compartment

The moderately high Henry's Regulation Consistent (232 Pa.m^3/mol) demonstrates that the essential expulsion instrument of styrene from water is volatilization.

9.3 Dividing to the Water Compartment

In case of a spill, styrene will gradually volatilize and little will break up. The focus to which amphibian creatures will be uncovered will rely upon the air and water temperature and disturbance. The exhaustion chart gives an outline of the difference in the styrene fixation with time, both in stale water and when blended gradually.

9.4 Parceling to the Dirt Compartment

In light of its low water solvency and the extent of its natural carbon parceling coefficient (determined Koc= 260-550), the versatility of styrene in soil is viewed as moderate to low. Taking into account the bioconcentration factor (BCF) for fish and the octanol/water Bioaccumulation, Development and Parceling segment coefficient.

9.5 Fire Concealment

Fires including styrene can be securely smothered with froth, dry powder, water mist or carbon dioxide. Nonetheless, water is definitely not a compelling quenching specialist for

The survey of the exceptionally broad writing prompts the accompanying ends:

Fluid styrene is aggravation to skin and eyes, while higher fume focuses might be irritant to the respiratory lot. Openness to styrene above as of now suggested working environment cutoff points might cause reversible effects on the sensory system. The cancer-causing chance to people is exceptionally low assuming suggested word related openness levels are not exceeded.

9.6 Hindrance

9.6.1 Wellbeing and Quality

Polymer content in completed styrene is, above all else, significant from a quality assurance perspective, and gets the most elevated consideration since it very well might be a dictation that due to inadequate product security, a risky response is in progress. The base focuses for oxygen and inhibitor should be kept up with to prevent oxidative debasement and resulting (poly)peroxide arrangement. Ordinarily 4-tertiary butyl catechol (TBC) is utilized for restraint, yet hydroquinone functions also. Since both require oxygen for their proper working, styrene is put away under air or Bert gas with adequate oxygen to guarantee a small mum substance in the fluid stage. In a new report on restraint science, it has been affirmed that free peroxide revolutionaries, benzaldehyde and formaldehyde are framed simultaneously. With 5%-vol. oxygen in the fume phase, more than adequate oxygen will be accessible for hindrance of the fluid stage. This implies that limited openness to air is the most ideal way to keep the oxygenates content as low as could be expected.

It ought to be noticed that at specific scopes, because of encompassing temperature varieties, styrene correspondence on the rooftop, walls and interior fittings of capacity tanks. Because of the great limits of the inhibitors, the re-condensed styrene contains no inhibitor. Safety measures should be taken to prevent polymer develop on the uncovered surfaces tank over the surface level of the fluid, of the tank, particularly on the tension vacuum valve.

In warm environments thought can be given to covering the inward surfaces of tanks, on the grounds that iron consumes oxygen and subsequently will variety styrene, and furthermore to keep away from polymer develop in the headspace of the tank. In US patent 4.161.554 a covering framework is portrayed, which contains TBC, and which has a presentation, from one application, expected to keep going for quite a long time. Further a fundamental Tenace and investigation plan is suggested which incorporates auxiliaries such as a fume return line and wellbeing valves.

CHAPTER 10

HAZARD AND SAFETY STUDY

10 Introduction:

HAZOP study is the investigation of potential risks involved in a process and its equipment which can be dangerous to the staff and the surrounding environment. It is a complete analysis of the plant safety and understanding which equipment need more care and attention while in running phase.

10.1 Fundamental Steps of HAZOP analysis:

- Divide the plant structure into sections and analyses the problems that may occur.
- Understand the reason of the problem and get to conclusion on the bases of the results.
- Discover what can be done for the problem to not reoccur.
- Pre plan few activates to cover up the problem.
- Record your findings.
- Repeat the process.

10.2 HAZOP on Reactor:

HAZOP of an adiabatic reactor using steam includes the disturbance in the reactor due to the flow of steam. As steam is also a heating medium and lower the vapor pressure of Ethyl Benzene to achieve a greater conversion rate.

10.3 HAZOP Analysis of a Liquid-Gas Separator:

A Hazard and Operability (HAZOP) analysis is a systematic method for identifying and evaluating the potential hazards and operability problems associated with a process or system. The HAZOP analysis of a Liquid-Gas Separator involves the following parameters:

Inlet Feed:

Overpressure of the inlet stream

High flow rate or velocity leading to erosion.

Contamination of feed with corrosive or toxic substances

Inadequate inlet flow control

Separation Chamber:

Overpressure in the vessel

High temperature or pressure leading to structural failure

Inadequate separation efficiency due to design flaws

Inadequate liquid level control leading to carryover

Gas Outlet:

Pressure surges causing damage to downstream equipment

Presence of flammable or toxic gases in the gas outlet stream

Inadequate gas flow control leading to choking or flashing

Corrosion of the gas outlet line

Liquid Outlet:

Presence of hazardous or toxic chemicals in the liquid outlet stream

Inadequate liquid flow control leading to carryover or flooding

Corrosion of the liquid outlet line

Inadequate level control leading to overflow.

Safety Report:

The Liquid-Gas Separator is an essential component of many industrial processes, and it is essential to ensure that it operates safely and reliably. The following safety recommendations should be considered when designing, installing, and operating a Liquid-Gas Separator:

10.4 HAZOP Study Report on Petlyuk Distillation Column

Introduction:

A Hazard and Operability (HAZOP) study is a systematic and structured approach to identifying potential hazards and operability issues in a process. The purpose of this HAZOP study is to identify and assess potential hazards associated with the operation of a Petlyuk Distillation Column.

HAZOP Analysis: The HAZOP study was conducted by examining each parameter of the Petlyuk Distillation Column and identifying potential hazards associated with it. The following parameters were analyzed:

Feed Inlet: The feed inlet to the column can potentially cause a hazard if the feed contains impurities or if the feed rate is too high, causing flooding of the column. To mitigate this, a feed pre-treatment system can be installed to remove impurities, and the feed rate can be controlled through the use of flow meters and control valves.

Heat Exchanger: The heat exchanger is an integral part of the Petlyuk Distillation Column and can pose a hazard if it fails due to overheating or pressure buildup. To prevent this, the heat exchanger can be equipped with temperature and pressure sensors, and a safety relief valve can be installed to prevent pressure buildup.

Tray Design: The tray design can potentially cause a hazard if the trays become clogged or if the tray spacing is not adequate. To prevent this, the tray design can be optimized to ensure proper spacing and to prevent clogging.

Reboiler: The reboiler can pose a hazard if it fails due to overheating or pressure buildup. To prevent this, the reboiler can be equipped with temperature and pressure sensors, and a safety relief valve can be installed to prevent pressure buildup.

Column Overhead: The column overhead can pose a hazard if it contains flammable or toxic gases. To prevent this, the column overhead can be equipped with gas detectors, and a ventilation system can be installed to remove any harmful gases.

Safety Report: Based on the HAZOP study, the following safety measures are recommended for the safe operation of the Petlyuk Distillation Column:

Regular maintenance and inspection of the column should be performed to ensure that all components are in good working condition.

A safety relief valve should be installed on the heat exchanger and the reboiler to prevent pressure buildup.

A gas detector and ventilation system should be installed on the column overhead to remove any harmful gases.

The feed inlet should be equipped with a pre-treatment system to remove impurities, and the feed rate should be controlled through the use of flow meters and control valves.

The tray design should be optimized to ensure proper spacing and to prevent clogging.

Conclusion: In conclusion, the Petlyuk Distillation Column is a complex process that requires careful analysis and safety measures to ensure safe and efficient operation. By conducting a HAZOP study and implementing the recommended safety measures, the risk of potential hazards can be minimized, and the safety of personnel and equipment can be ensured.

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