Kurdistan Region
Salahaddin University-Erbil
College of Engineering
Chemical-Petrochemical Engineering Department

STYRENE PRODUCTION

A Project Submitted to the Chemical-Petrochemical Engineering Department

University of Salahaddin-Erbil

in the Partial Fulfillment of the Requirement for the Degree of Bachelor of Science

in Chemical-Petrochemical Engineering

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2024-2025

Abstract

The production of styrene is a critical process in the petrochemical industry, driven by the increasing demand for polymers such as polystyrene, ABS, and SAN. This project focuses on the design and optimization of a styrene production plant through the catalytic dehydrogenation of ethylbenzene. The process is evaluated in terms of material and energy balances, equipment design, and process control, aiming to achieve a styrene purity of 99% with minimal by-products. Alternative methods such as propylene oxide, butadiene, and pyrolysis gasoline routes are also discussed and compared based on efficiency, cost, and environmental impact. Detailed calculations for the reactor, distillation columns, and heat exchangers are conducted to ensure optimal performance and energy integration. The findings underscore the importance of process optimization to enhance styrene yield, reduce energy consumption, and minimize waste generation, providing a comprehensive framework for sustainable chemical engineering practices.

Acknowledgment

I would like to extend my heartfelt gratitude to Mr. Ahmed Omer, our project supervisor, for his steadfast support throughout this journey. His consistent guidance, insightful feedback, and encouragement were instrumental in the successful completion of this research.

My sincere thanks also go to the Head of the Department of Chemical and Petrochemical Engineering, along with the entire faculty, for their continuous support and motivation during our academic path. Their passion for teaching and commitment to excellence have been truly inspiring.

I am especially thankful to my family for their unwavering encouragement and the sacrifices they have made. Their faith in me has been a constant source of strength and motivation.

This research is the product of dedication and perseverance, and we take great pride in its completion. We hope it serves as a valuable contribution to our field of study.

Supervisor’s Certificate

I certify that the engineering project titled " STYRENE PRODUCTION” was done under my supervision at the Chemical-Petrochemical Engineering Department, College of Engineering - Salahaddin University–Erbil. In the partial fulfillment of the requirement for the degree of Bachelor of Science in Chemical-Petrochemical Engineering

Contents

List of figures

List of tables

Nomenclature

A-Heat capacity coefficient

ACP – Acetophenone

B – By-product stream (kg/hr)

B – Antoine Equation Constant

C – Antoine Equation Constant

C1 – Heat Capacity Coefficient (First Coefficient)

C2 – Heat Capacity Coefficient (Second Coefficient)

C3 – Heat Capacity Coefficient (Third Coefficient)

C4 – Heat Capacity Coefficient (Fourth Coefficient)

Cp – Specific heat capacity (kJ/kg·K)

D – Distillation column

EB – Ethylbenzene (C_8H_{10})

EBHP – Ethylbenzene hydroperoxide

EPS – Expanded Polystyrene

F – Feed stream (kg/hr)

G – Gas stream (kg/hr)

H – Enthalpy (kJ)

L – Liquid phase

M – Methane (kg/hr)

MBA – Methylbenzyl alcohol

NG – Natural Gas

P – Product stream (kg/hr)

PO – Propylene oxide

PyGas – Pyrolysis Gasoline

Q – Heat duty (kJ/hr)

$\alpha - relative\ volatility$

R – Recycle stream (kg/hr)

S – Styrene (C8H8)

SAN – Styrene-Acrylonitrile

SBR – Styrene-Butadiene Rubber

T – Toluene (C7H8)

Tc – Critical temperature (K)

V – Vapor stream

VCH – 4-vinylcyclohexene

W – Wastewater stream (kg/hr)

X1 – Conversion factor of Ethylbenzene to Styrene

X2 – Conversion factor of Ethylbenzene to Toluene

Chemical Compounds:

C2H4 – Ethylene

C2H6 – Ethane

C67H8 – Toluene

C6H6 – Benzene

C8H8 – Styrene

C8H10 – Ethylbenzene

CH4 – Methane

H2 – Hydrogen

H2O – Water

Units of Measurement:

g/cm^3 – Gram per cubic centimeter

kJ – Kilojoule

kg/hr – Kilogram per hour

kmol – Kilomole

mPa.s – Millipascal second

°C – Degrees Celsius

atm – Atmosphere

K – Kelvin

1 Chapter one: Introduction

1.1 Background

Styrene, also known by various names such as ethenylbenzene, vinylbenzene, cinnamene, and phenylethene, is an organic compound widely used in the chemical industry. Its chemical formula is C_8H_8 and structure formula is $C_6H_5CH = CH_2$, consisting of a benzene ring attached to an ethylene group. Styrene is a colorless to slightly yellow liquid with a sweet, aromatic odor at room temperature, highly flammable and can form explosive mixtures with air, is primarily used as a monomer in the production of various polymers and copolymers, playing a crucial role in the plastics and rubber industries. It is the key building block for manufacturing polystyrene (PS), one of the most widely used thermoplastics, known for its lightweight and insulating properties. Additionally, styrene is used in the production of acrylonitrile-Butadiene-Styrene (ABS), Styrene-Butadiene Rubber (SBR), Styrene-Acrylonitrile (SAN), Expanded Polystyrene (EPS). The chemical structure of the styrene is shown in the figure 1.1[1], [2]

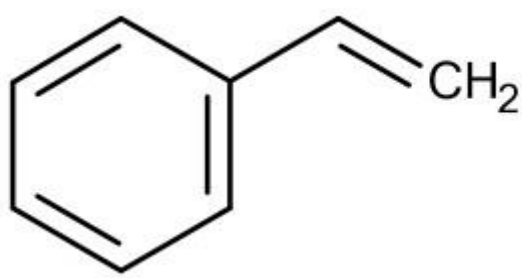


Figure 1.1-1 / styrene structure

Styrene is commercially produced via two main routes: dehydrogenation and coproduction with propylene oxide, both using ethylbenzene as an intermediate from benzene and ethylene. Over 50% of commercial benzene is consumed in this process. Most ethylbenzene and styrene plants operate under licensed technologies with modest fees. As a widely traded commodity, styrene must meet a minimum purity of 99.8%, achievable in modern plants. Some producers invest in higher purity (99.95%) for a competitive edge, with advancements making such production increasingly routine. [3]

1.2 History

Styrene was discovered in the 19th century by Eduard Simon through the distillation of storax, but it had no commercial applications due to the brittleness of its polymers. In the 1930s, I.G. Farben and Dow Chemical developed efficient dehydrogenation processes. During WWII, styrene became essential for synthetic rubber production, later shifting mainly to polystyrene, which now accounts for about 65% of its consumption. U.S. production grew from 2.0 million metric tons in 1970 to 5.8 million in 2004. Its popularity is due to easy handling, polymerization capability, raw material availability (benzene and ethylene), and advancements in manufacturing that reduced costs and enabled large-scale production.[2], [4]

1.3 Uses of styrene

Styrene monomer serves as a crucial raw material in the production of various polymer-based products, including thermoplastics, elastomers, dispersions, and thermoset plastics.

- About 65% of the styrene produced is used to manufacture polystyrene.
- Around 6% is directed into the production of styrene-butadiene rubber (SBR).
- Approximately 7% is utilized in the production of styrene-butadiene latex.

- Roughly 9% is used in styrene-acrylonitrile (SAN) copolymers and ABS (acrylonitrile-butadiene-styrene) terpolymers.
- An additional 7% is combined with unsaturated polyester resin to produce materials used in fiberglass-reinforced boats and storage tanks.
- The remaining styrene is used in a variety of applications, including blends with other thermoplastics for an expanding range of products, such as ion exchangers and adhesives.[5]

1.4 physical properties

Table 1-1 physical properties of styrene[4]

Chemical Formula	C_8H_8
Molecular weight	104.15 g/mol
Liquid density	0.906 g\L at 20 ℃
Vapor pressure	12.4 mm Hg
Form at room temperature	liquid
Color	colorless
Liquid heat capacity	151.29 (J/mol*K)
Melting point	-30 ℃
Corrosivity	Noncorrosive to metals except to copper and alloys of copper.
Boiling point	145 ℃
Flash point	31.14 ℃
Solubility in water	0.3 g\L (20℃)
Conductivity	0.035 (W/m*K)
Viscosity	0.695 mPa.s

1.5 Chemical properties

1.5.1 Polymerization

The polymerization of styrene (C_8H_8) is a well-studied process that produces polystyrene, a widely used thermoplastic polymer. This reaction typically proceeds via free-radical polymerization, which involves three main stages: initiation, propagation, and termination.

- Initiation: The reaction begins with the decomposition of an initiator (e.g., benzoyl peroxide) to generate free radicals.

$$Initiator \rightarrow Free\ radical$$

$$Free\ radical + Styrene \rightarrow New\ free\ radical$$

- Propagation: The free radical reacts with more styrene molecules repeatedly, causing the polymer chain to grow.

$$\text{Free radical} + \text{Styrene} \rightarrow \text{Longer polymer chain}$$

- Termination: The polymerization process ends when two radical chains combine, forming a stable polymer.

$$Polymer\ chain + Polymer\ chain \rightarrow Stable\ polymer\ (Polystyrene)$$

1.5.2 Oxidation

Styrene oxidation introduces oxygen-containing groups (e.g., epoxides, aldehydes, carboxylic acids) into the styrene molecule (C_8H_8) $this\ occures$ at the vinyl group or aromatic ring, depending on the oxidizing agent (e.g., $KMnO_4$, O_3, H_2O_2) .

- Epoxidation: Styrene reacts with peracids (e.g., mCPBA) to form styrene oxide (an epoxide).

$$Styrene\ +\ Peracid\ \rightarrow\ Styrene\ Oxide$$

- Cleavage of the Double Bond: Strong oxidants like $KMnO_4$ or O_3 cleave the double bond, producing benzoic acid and formic acid.

$$Styrene\ +\ [O]\ \rightarrow\ Benzoic\ Acid\ +\ Formic\ Acid$$

- Hydroxylation: Styrene can be hydroxylated to form 1,2-diols (e.g., using OsO_4 or H_2O_2).

$$Styrene\ +\ [O]\ \rightarrow\ 1{,}2-Diol$$

1.5.3 Halogenation

The halogenation of styrene is an electrophilic addition reaction in which halogens (e.g., chlorine Cl_2 or bromine Br_2) are added to the double bond (C=C) in the vinyl group ($–CH=CH_2$) of styrene (C_8H_8). This reaction produces 1,2-dihaloethylbenzene (e.g., 1,2-dibromoethylbenzene when using bromine). The reaction typically occurs at room temperature in an inert solvent (e.g., CCl_4) and does not require a catalyst.

1.5.4 Hydrogenation

Styrene can be hydrogenated to produce ethylbenzene, and sometimes to produce toluene and methane.

1.5.5 Reactions with Acids and Bases

The vinyl group in styrene can participate in addition reactions with strong acids, such as HCl or HBr, leading to the formation of corresponding adducts. [4], [6]

2 Chapter two: production methods

2.1 sources of styrene:

The raw materials used in making styrene are obtained from crude oil or liquified petroleum gas (LPG). A range of processes are in- volved in transforming crude oil or gas into styrene.

The material that obtained from crude oil and LPG are:

1. Ethylbenzene is typically obtained from crude oil through a process known as alkylation of benzene with ethylene.
2. Toluene ($C_6H_5CH_3$) (Alternative Route): Obtained from crude oil and can be used to produce benzene via hydrodealkylation or directly converted into styrene via alkylation with methanol.
3. Naphtha: naphtha is a critical material in the petrochemical industry, acting as the primary source of benzene and ethylene, which are essential for producing styrene.
4. Ethane (C_2H_6): Ethane can be obtained from LPG and used as a feedstock for ethylene production. Ethylene is then used to produce ethylbenzene, the key precursor to styrene.
5. Butadiene: Butadiene can be transformed into benzene through a process known as Diels-Alder cycloaddition, once you have benzene, ethylbenzene can be synthesized by reacting it with ethylene, and then we can produce styrene.[1]

2.2 production methods

Styrene is the precursor to polystyrene and several copolymers. Approximately 25 million tons of styrene were produces in 2010. There are many methods in producing Styrene which are: -

2.2.1 styrene from propylene oxide

the first step is direct air oxidation of ethyl benzene at 130 c and 0.2mpa. this gives ethylbenzene hydroperoxide (EBHP) and methylbenzyl alcohol (MBA) and acetophenone (ACP), by the following reacting over molybdenum as catalyst.

$$C_8H_{10} + O_2 \rightarrow \; C_6H_5CH(OOH)CH_3 \qquad \text{EBHP}$$

$$C_8H_{10} + \frac{1}{2}O_2 \rightarrow C_6H_5CH(CH_3)OH \qquad \text{MBA}$$

$$C_8H_{10} + xO_2 \rightarrow \quad C_6H_5CO(CH_3) + acids \quad \text{(ACP)}$$

Conversion is about 13%. the selectivity of ethylbenzene to EBHP is 90% and the selectivity to MBA and ACP is 5-7% Ethylbenzene hydro peroxide is then reacted with propylene at 110c and 4 MPa in the presence of titanium as catalyst to form propylene oxide (PO) and MBA by the following reaction

$$C_6H_5CH(OOH)CH_3 + C_3H_6 \rightarrow C_3H_6O + C_6H_5CH(CH_3)OH$$

To improve yields, acetophenone (ACP) is hydrogenated to α-methylbenzyl alcohol (MBA) in the liquid phase at 90–150°C and 8 MPa, using a ZnO and CuO catalyst. About 90% of ACP is converted, with 92% selectivity to MBA.by the following reaction.

$$C_6H_5CO(CH_3) + H_2 + C_6H_5CH(CH_3)OH$$

Finally, the MBA is dehydrated to styrene at 250°C and low pressure over AL2O3 by the following reaction.

$$C_6H_5CH(CH_3)OH \rightarrow C_6H_{5CH} = CH_2 + H_2\mathrm{O}$$

2.2.2 Styrene from butadiene

In this process 1,3 butadiene is converted to 4-vinylcyclohexene(VCH) at 0-80c° and 0.1-1.3 MPa over nitrosyl halide-iron complex as catalyst by the following reaction

$$2C_4H_6 \rightarrow C_6H_9CH = CH_2 \quad (VCH)$$

is then dehydrogenated to styrene by the following reaction

$$C_6H_9 = CH_2 \rightarrow C_6H_5CH = CH_2 + H_2$$

2.2.3 Styrene from toluene

Monsanto worked extensively on a process for styrene starting with air oxidation of toluene to give stilbene. This used a fluidized bed of supported lead oxide catalyst

$$2C_6H_5CH_3 + O_2 \rightarrow C_6H_5CH = CHC_6H_5 + H_2O$$

Stilbene is then reacted with ethylene over molybdenum catalyst to give styrene

$$C_6H_5CH = CHC_6H_5 + C_2H_4 \rightarrow C_6H_5CH = CH_2$$

2.2.4 Catalytic Dehydrogenation of Ethylbenzene

The direct dehydrogenation of ethylbenzene to styrene produces 85% of commercial styrene. It occurs in the vapor phase with steam over an iron oxide-based catalyst. The reaction is endothermic and can be carried out adiabatically or isothermally.

The primary reaction involves the reversible and endothermic transformation of ethylbenzene into styrene and hydrogen.

$$C_6H_5CH_2CH_3 \leftrightarrow C_6H_5CH = CH_2 + H_2$$

2.2.5 Styrene from Pyrolysis Gasoline (PyGas)

PyGas, a byproduct of ethylene production, is rich in aromatics like ethylbenzene, which is the key precursor for styrene. The process involves extracting ethylbenzene and converting it to styrene through dehydrogenation at high temperatures using a catalyst. Steam is used to enhance the reaction and prevent coke formation. The final styrene product is purified and stabilized to prevent polymerization.

This method efficiently utilizes byproducts, reducing costs and improving resource efficiency. However, challenges include complex separation, catalyst deactivation, and coke formation, requiring precise process control.[4]

2.3 Selection of manufacturing process

We select ethylbenzene dehydrogenation process because

1- Its modern process.
2- less byproduct.
3- high yield of styrene about 93%.
4- lower cost.

2.4 Equipment description

Fired Heater H-1: The fired heater heats the low-pressure steam to any temperature. H-1 is fueled with natural gas (NG).

Heat Exchangers: Heat exchanger E-1 heats the ethylbenzene feed, recycled stream.

Heat exchanger E-2 may be used to cool the reactor outlet.

Catalytic Reactor R-1: This a fixed-bed reactor with a heat-transfer jacket.

Three-Phase Separator V-1: The reactor outlet enters the three-phase separator, it passes through an inlet device (such as a diverter) to distribute the flow evenly, and separates the mixture to 3 products, gas product (hydrogen and methane), liquid product which contains toluene, EB and styrene which is then fed to distillation towers, and bottom product (wastewater).

Distillation Columns T-1 and T-2: From the three-phase separator, the organic liquid product stream enters the distillation. The columns operate at or below the normal boiling point of styrene at the desired column outlet pressure. To eliminate significant polymerization of styrene, the distillation units are operated at a moderate vacuum to keep the temperature low. the top product from the toluene column T-1, must contain at least 95% of the toluene entering the distillation train, and must contain 99% toluene, with the rest being ethylbenzene. the bottoms product from the toluene column (T-1), is further distilled in the ethylbenzene-recycle column (T-2). The overhead ethylbenzene product contains small amounts of toluene and styrene and is recycled to mix with the feed before the reactor. The bottoms product of T-2, must be 99% pure styrene.

Mixers: The mixer receives multiple input streams, which could include reactants, solvents, or recycled process streams. It ensures uniform mixing to achieve proper composition before entering the reactor.

Condensers: Condensers remove heat from vapor, converting it into a liquid phase. They are mainly used in distillation columns.

Reboilers: Reboilers supply heat to a distillation column to generate vapors that help separate components. They provide the necessary boiling action at the column base.

2.5 comparison between methods

Table 2-1 Comparison between methods

Method	Reaction	Advantage	Disadvantage
Catalytic Dehydrogenation of Ethylbenzene	Ethylbenzene is heated in the presence of iron oxide-based catalysts to remove hydrogen and produce styrene.	Clean process, ideal for continuous production, High selectivity and yield.	Requires high temperatures (600-650°C), consumes significant energy, and hydrogen removal can be costly.
Styrene from Propylene Oxide (PO)	Ethylbenzene undergoes oxidation to form ethylbenzene hydroperoxide, which reacts with propylene oxide to produce an alcohol that is then dehydrated to styrene.	• High-quality styrene product. • Efficient process with good selectivity. • Fewer side products.	• High cost of propylene oxide as a feedstock. • Requires high energy input for the reaction. • Relatively less common compared to other methods.
Styrene from Butadiene	Butadiene undergoes hydroformylation (reaction with CO and H2) followed by dehydrogenation to produce styrene.	• Uses readily available butadiene, which is often a by-product of other petrochemical processes.	• Lower selectivity compared to other methods. • Multi-step process, which makes it more complex and costly.

Styrene from Toluene	Toluene undergoes alkylation with ethylene or is dehydrogenated to form styrene.	• Toluene is an inexpensive and readily available feedstock. • The process can have fewer by-products, improving product purity.	• Requires high temperatures (around 600°C) for dehydrogenation, leading to high energy consumption. • Catalyst costs can be high, and catalyst deactivation can reduce efficiency. • Alkylation step can be complex.
Styrene from Pyrolysis Gasoline (PyGas)	Pyrolysis gasoline, a by-product from steam cracking of hydrocarbons, is used to produce styrene via catalytic reforming or dehydrogenation.	• Uses pyrolysis gasoline, a by-product from other petrochemical processes, reducing waste. • Can be integrated into existing petrochemical complexes.	• PyGas is a mixture, so it may contain impurities that complicate the process. • Process efficiency may be lower due to the variable composition of PyGas. • Catalyst requirements and feedstock separation may increase costs.

Process Description

The process begins with ethylbenzene, which is preheated in E-2 until it reaches saturated vapor. This vapor is then mixed with steam from the fired heater E-1. Steam plays a crucial role in the process by Providing the heat required for the reaction, acting as an inert diluent to shift the reaction equilibrium toward styrene production, limiting side reactions and reducing coke formation on the catalyst, thereby extending its lifespan, The steam to ethylbenzene ratio entering R-1 in Stream 6 ranges between 6 and 12. In reactor R-1 the process uses a proprietary iron catalyst that minimizes (but does not eliminate) side reactions at higher.

The main reaction occurring in R-1 is:

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

(Ethylbenzene → Styrene + Hydrogen)

This endothermic and reversible reaction takes place at high temperatures (800–950 K) and low pressures to maximize styrene yield. The reaction approaches 80% of equilibrium, using a proprietary iron-based catalyst that minimizes side reactions.

Several undesired side reactions occur, leading to byproducts and reduced yield:

- Thermal Cracking of Ethylbenzene: Ethylbenzene can decompose into benzene and ethylene

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

- Carbon Formation (Coking): Ethylbenzene can degrade further to form carbon (coke) and hydrogen

$$C_8H_{10} \rightarrow 8C + 5H_2$$

Carbon deposition on the catalyst surface can poison the catalyst, reducing its activity.

- Hydrogenation of ethylbenzene: ethylbenzene can react with hydrogen to form toluene and methane

$$C_8H_{10} + 2H_2 \rightarrow C_7H_8 + CH_4$$

This reaction reduces the yield of styrene.

The reactor effluent is cooled in E-3, before entering a three-phase separator (V-1), Bottom phase is wastewater, which requires further treatment before disposal, Top phase: Light gases (methane & hydrogen), which can be used as fuel, Liquid phase: Contains toluene, ethylbenzene, and styrene. undergoes distillation in T-1 and T-2, T-1 removes most toluene in overhead, The remaining mixture is separated in T-2, the top product of T-2 (ethylbenzene, toluene, and styrene) is recycled back to the reactor. Bottom Stream of T-2 (styrene with trace ethylbenzene & toluene) is the final product. For simplicity, assume that the only side reaction that occurs in R-1 is the hydrogenation of ethylbenzene to form toluene and methane.

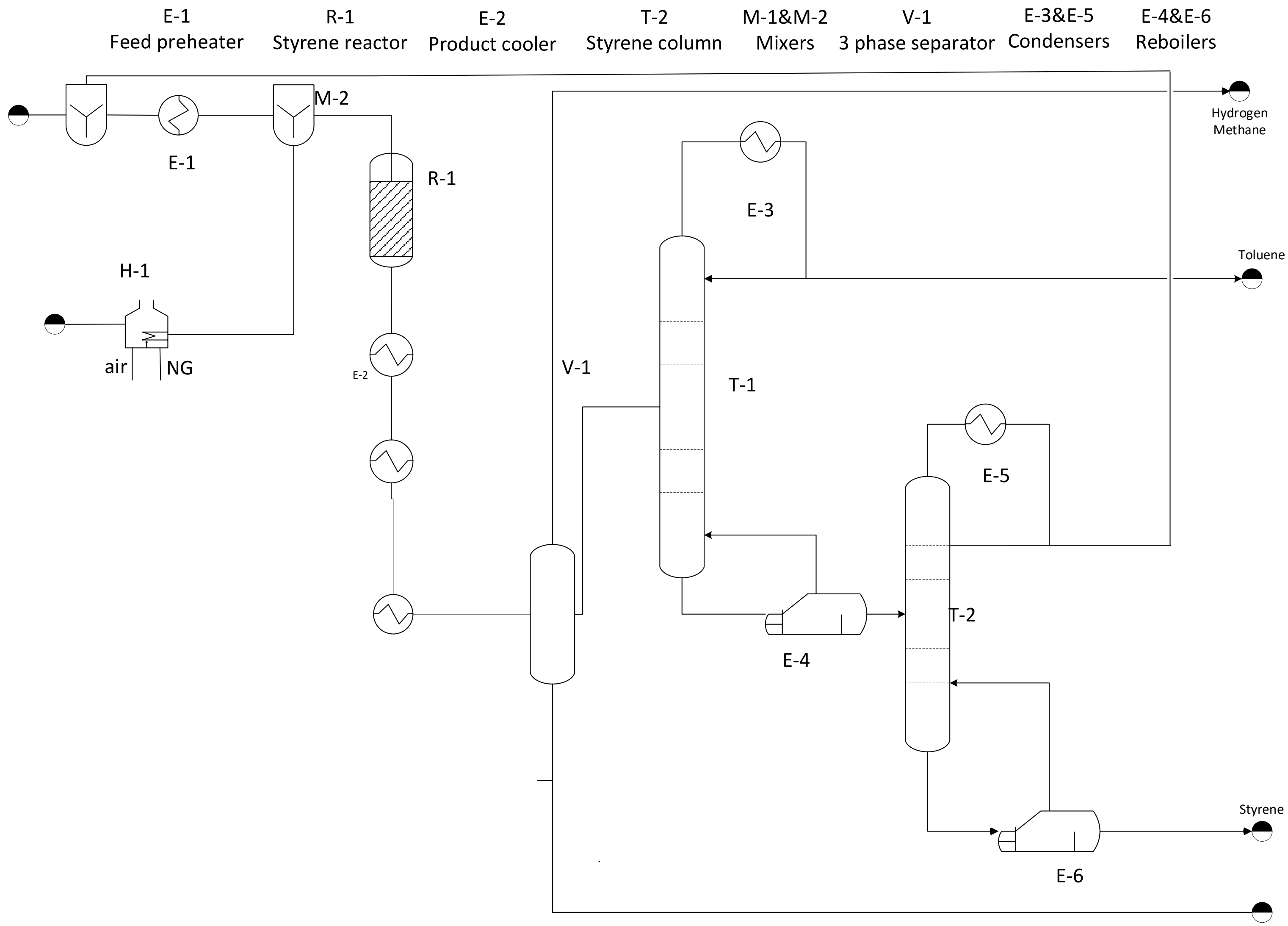


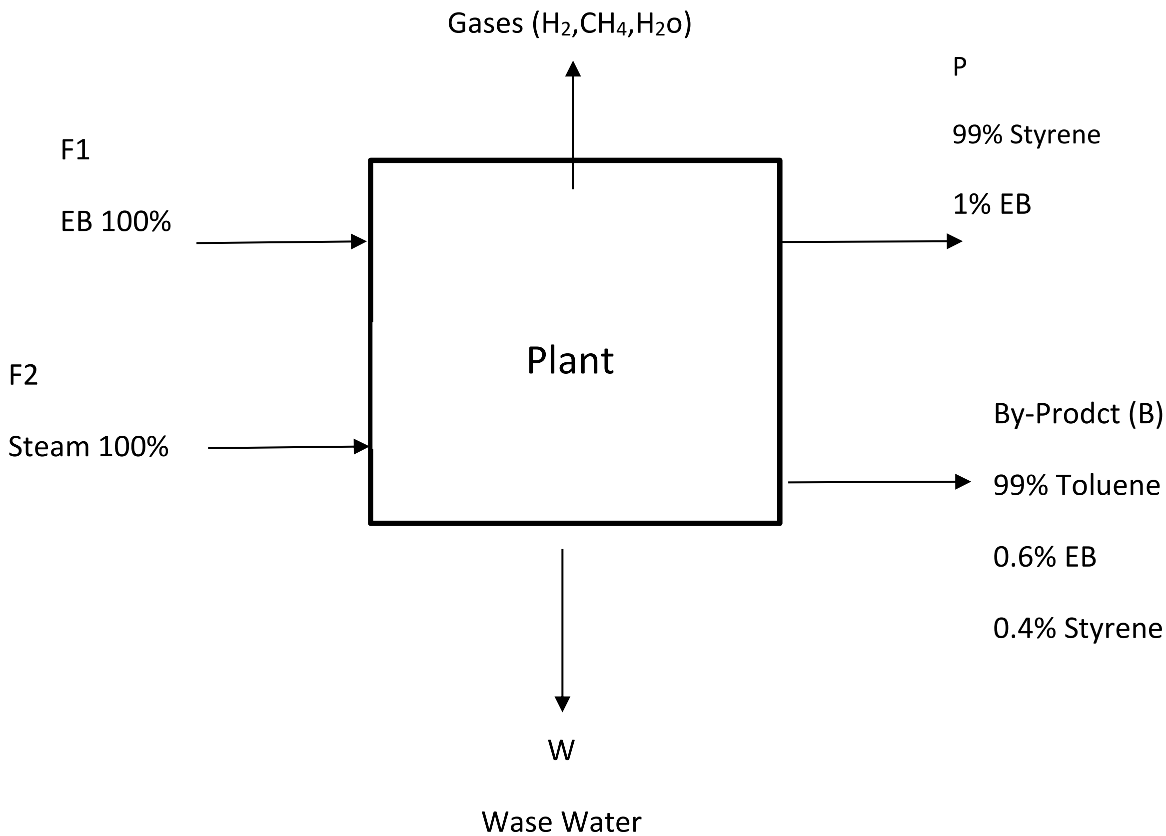
Table 2-2"PFD of styrene production"

2.6 physical properties of raw materials and by-products

Table 2-3 physical properties of raw materials and by-products

Materials	Chemical formula	viscosity	Melting point	Boiling point	Flash point	density
ethylene benzene	C_8H_{10}	0.65 mPa·s at 25°C	-95°C	136°C	15°C (closed cup)	0.867 g/cm³ at 20°C
Ethylene	C_2H_4	0.1 mPa·s at 0°C	-169.2°C	-103.7°C	-136°C	1.18 kg/m³ at 0°C
Benzene	C_6H_6	0.65 mPa·s at 25°C	5.5°C	80.1°C	-11°C	0.8765 g/cm³ at 20°C
Toluene	$C_6H_5CH_3$	0.59 mPa·s at 25°C	-95°C	110.6°C	4.4°C	0.867 g/cm³ at 20°C
Ethane	C_2H_6	0.101 mPa·s at 0°C	-182.8°C	-88.6°C	-135°C	1.3562 kg/m³ at 0°C
Methane	CH_4	0.0112 mPa·s (at 0 °C)	-182.5°C	-161.5°C	-188°C	0.657 kg/m³ (at 0°C)
Hydrogen	H_2	0.0089 mPa·s(at 0 °C)	-259.16°C	-252.87°C	Not applicable	0.0899 kg/m³ (at 0°C)

3 Chapter three: material balance



3.1 Overall material balance.

F1 + F2 = W +B + P + Gases

Capacity $= 80000\ \frac{ton}{year}$

Typical operating time for chemical plant is 300 $\frac{days}{year}$

So 80000 $\frac{ton}{yr} \times \frac{100kg}{ton} \times \frac{1yr}{300day} \times \frac{day}{24hr}$

P=11111.11$\frac{kg}{hr}$

3.2 Overall balance on components:

1.$C_8H_{10} \rightleftarrows C_8H_8 + H_2$ main reaction

2.$C_8H_{10} + H_2 \rightarrow C_7H_8 + CH_4$ Side reaction

Product of styrene = P Kg/hr

(Consist of 99 wt% C8H8 and 1 wt% C8H10)

By product =B Kg/hr (Consist of 99wt% C7H8 0.6wt% C8H10 and 0.4wt% C8H8) [7]

Overall mole balance on C_8H_{10} (EB)

In − reacted = out

$$\frac{F1}{106} - \frac{(F1X1 + F1X2)}{106} = \frac{0.006B}{106} + \frac{0.01P}{106}$$

$F_1 - F_1X_1 - F_1X_2 = 0.006B + 0.01P$

$F_1(1 - X_1 - X_2) = 0.006B + 0.01P$

$F_1(1 - X_1 - X_2) = 0.006B + 0.01(11111.11)$

$F_1(1 - X_1 - X_2) = 0.006B + 111.1111$ ……..(1)

M.B on C_8H_8:

In+produced = out

$$0+\frac{F1X1}{106}=\frac{0.004B}{104}+\frac{0.99P}{104}$$

F_1X_1 = 0.00407B+1.00904P

F_1X_1= 0.00407B+11211.55 ………(2)

M.B on C_7H_8(toluene):

In + produced = out

$$0+\frac{F1X2}{106}=\frac{0.99B}{92}$$

F_1X_2 = 1.141B ………..(3)

Selectivity of C_7H_8=0.06 [7]

$$0.06=\ \frac{kmol\ of\ C7H8\ produced}{kmol\ of\ C8H8\ produced}=\frac{F1X2}{F1X1}$$

$X_2 = 0.06X_1$ ………….(4)

By sub (4) in (3)

$0.06F_1X_1$ = 1.141B

F_1X_1 = 19.017B ………..(5)

And by sub (5)in (2)

19.017 = 0.00407B+11211.55

B(19.017−0.00407) = 11211.55

$B = \frac{11211.55}{19.01293} = 589.68\frac{kg}{h}$

Now from (5) $F_1X_1 = 19.017B$

$F_1X_1 = 19.017(589.68)$

$F_1X_1 = 11213.944\ \frac{kg}{h}$ ……….(6)

And from equ. (3) $F_1X_2 = 1.141B$

$F_1X_2 = 672.82\frac{kg}{h}$ ………(7)

From equ. (1) $F_1(1-X_1-X_2) = 0.006B+111.1111$

$F_1-F_1X_1-F_1X_2 = 0.006(589.68) +111.1111$

$F_1-11213.944-672.82 = 114.65$

$F_1 = 12001.4\frac{kg}{h}$

Now from (6) $F_1X_1 = 11213.944$

$X_1 = \frac{11213.944}{12001.41} = 0.934 = 93.4\%$

From (4) $X_2 = 0.006X_1 = 0.06(0.934)$

$X_2 = 0.056 = 5.6\%$

M.B on H_2:

In+produced-reacted = out

$$\frac{F1}{106} - \frac{F1X2}{106} = \frac{A}{2}$$

$$\frac{F1}{106}(X1 - X2) = \frac{A}{2}$$

$$\frac{12001.41}{106}(0.934 - 0.056) = \frac{A}{2}$$

$$\frac{A}{2} = 99.41$$

$$A = 198.82\frac{kg}{hr}$$

M.B on CH_4:

In + produced = out

$$\frac{F1X2}{106} = \frac{M}{16}$$

$$\frac{672.82}{106} = \frac{M}{16}$$

$$\frac{M}{16} = 6.35$$

M=101.6 $\frac{kg}{h}$

To determination flows of C_7H_8, C_8H_8 and C_8H_{10} in stream B

$C_7H_8 = 0.99B = 0.99(589.68) = 583.78\ \frac{kg}{h}$

$C_8H_8 = 0.004B = 0.004(589.68) = 2.36\frac{kg}{h}$

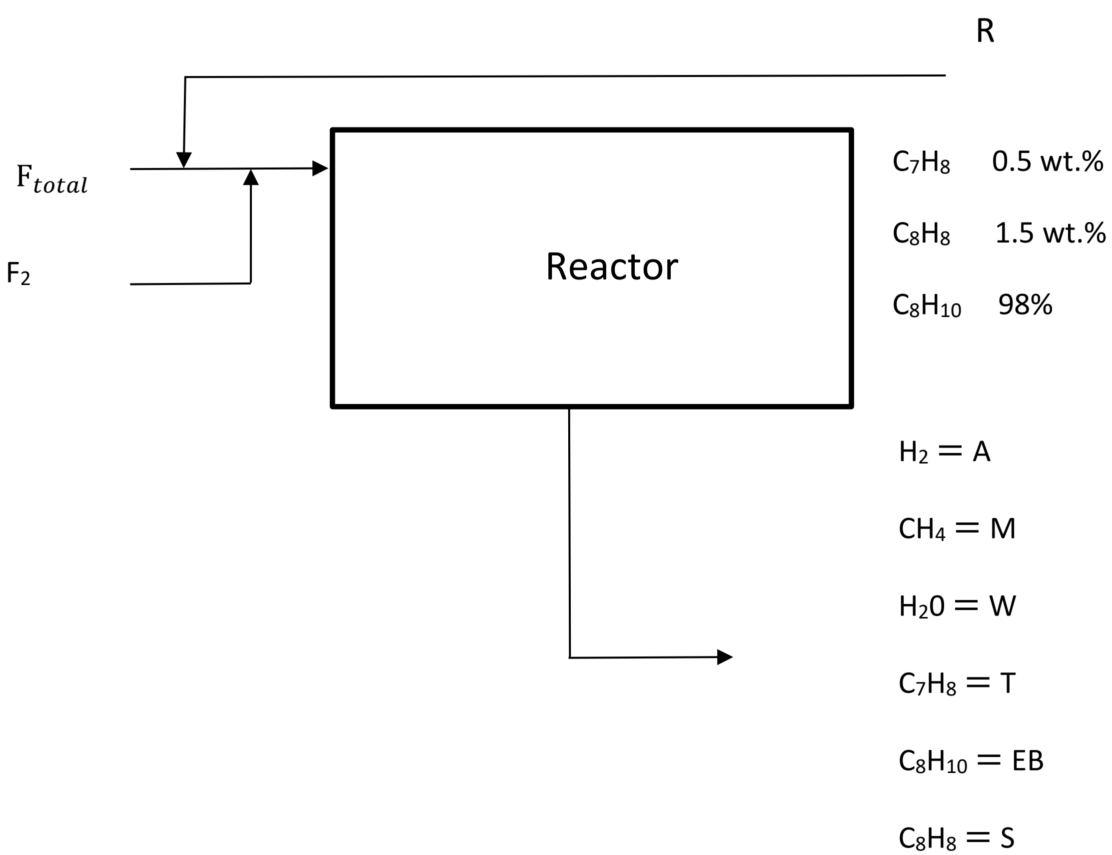
$C_8H_{10} = 0.006B = 3.54\frac{kg}{h}$

And for stream (P)

$C_8H_8 = 0.99P = 0.99(11111.11) = 10999.999\ \frac{kg}{h}$

$C_8H_{10} = 0.01P = 0.01(11111.11) = 111.1111\ \frac{kg}{h}$

3.3 Material balance on reactor:



Steam to EB mole ratio into the reactor is (6-12), so steam to EB ratio is 9 [7]

Single pass conversion = 0.65 = $\frac{C8H10\ reacted\ overall}{CH10\ in\ put\ to\ reactor}$ [7]

Total reacted EB = $F_1X_1 + F_2X_2 = F_1(X_1 + X_2)$

$\mathrm{T.\,r}_{EB}$ =12001.41(0.056 + 0.934) = T.r.EB = $11881.4\,\frac{kg}{h}$

C_8H_{10}(EB) input to the reactor = F_1 + 0.98R

Single pass conversion = $\frac{T.r.EB}{F1 + 0.98R}$

$0.65 = \frac{11881.4}{12001.41 + 0.98R}$ 7800.92 + 0.637R = 11881.4

0.637R = 4080.48 R = $6405.78\,\frac{kg}{h}$

$F_{total} = F_1 + R = 18407.2\,\frac{kg}{h}$

Component flow in R stream

$C_7H_8 \rightarrow 0.005(6405.78) = 32.03\frac{kg}{h}$

$C_8H_8 \rightarrow 0.98(6405.78) = 6277.66\frac{kg}{h}$

$C_8H_{10} \rightarrow 0.015(6405.78) = 96.1\frac{kg}{h}$

Steam EB inlet to the reactor 9:1

Total EB to reactor = F_1 + 0.98R

$12001.41 + 0.98(6405.78) = 18279.1\frac{kg}{h}$

$$\frac{18279.1\,\frac{kg}{h}}{106\,\frac{kg}{kmol}}$$

Total EB in to reactor =172.44 $\frac{kmol}{h}$

T EB = 172.44$\frac{kmol}{h}$

F_2= 9×172.44 = 1551.96 $\frac{kmol}{h}$

F_2 = 1551.96× 18 $\frac{kg}{kmol}$ = 27935.28 $\frac{kg}{hr}$

M.B on H2o in reactor:

In = out

F_2 = W

W = 27935.28$\frac{kg}{h}$

M.B on C_7H_8 in reactor:

In + produced = out

$\frac{0.005R}{92} + \frac{F1X2}{106} = \frac{T}{92}$

$$\frac{0.005R}{92} + \frac{F1X1}{106} = \frac{T}{92}$$

T = 616.4 $\frac{kg}{h}$

M.B on C_8H_8:

In + produced = out

$$\frac{0.015R}{104}+\frac{F1X1}{106}=\frac{S}{104}$$

$$\frac{96.1}{104}+\frac{11213.944}{106}=\frac{S}{104}$$

$$S = 11098.46\,\frac{kg}{h}$$

M.B on C_8H_{10}:

In − reacted = out

$$\frac{\text{(T.EB inlet to reactor)}}{106}-\frac{\text{(F1X1+F1X2)}}{106}=\frac{E}{100}$$

$$E=6397.7\frac{kg}{h}$$

M.B on H_2:

In + produced – reacted = out

$$0+\frac{F1X1}{106}-\frac{F1X2}{106}=\frac{A}{2}$$

$$\frac{F1(X1-X2)}{106}=\frac{A}{2}$$

$$\frac{12001.41(0.934-0.05)}{106}=\frac{A}{92}$$

$$A = 198.82\frac{kg}{h}$$

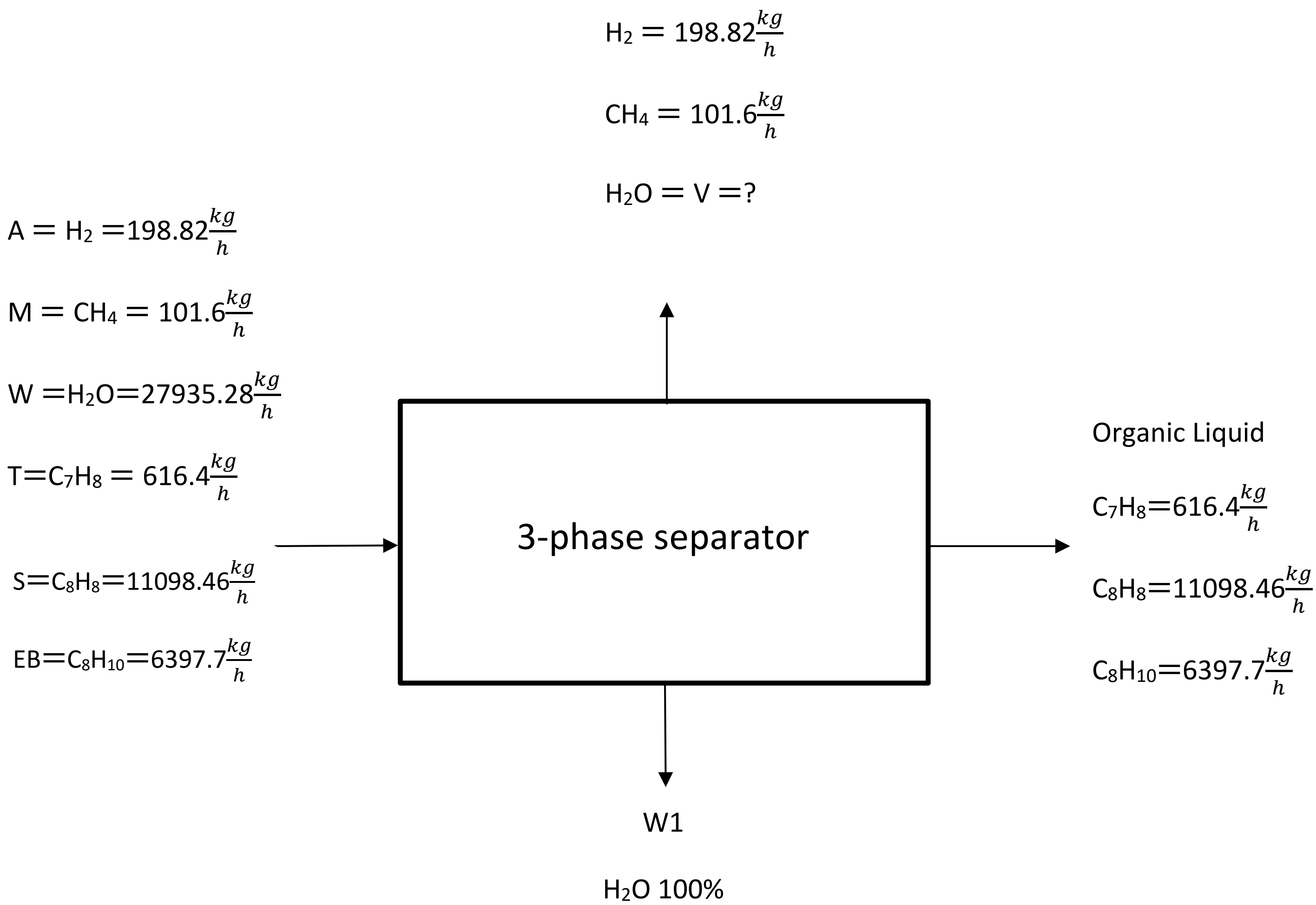
M.B on CH_4:

In + produced = out

$$0 + \frac{F1X2}{106} = \frac{M}{16}$$

$$M = 101.6\,\frac{kg}{h}$$

3.4 Material balance on three phase separator:



99.7% of water will removed from the heavy liquid stream

So $W_1 = W$ (in separator feed) $\times 99.7\%$

$W_1 = (27935.28)(0.997)$

$W_1 = 27851.474 \frac{kg}{h}$

M.B on H_2O in separator:

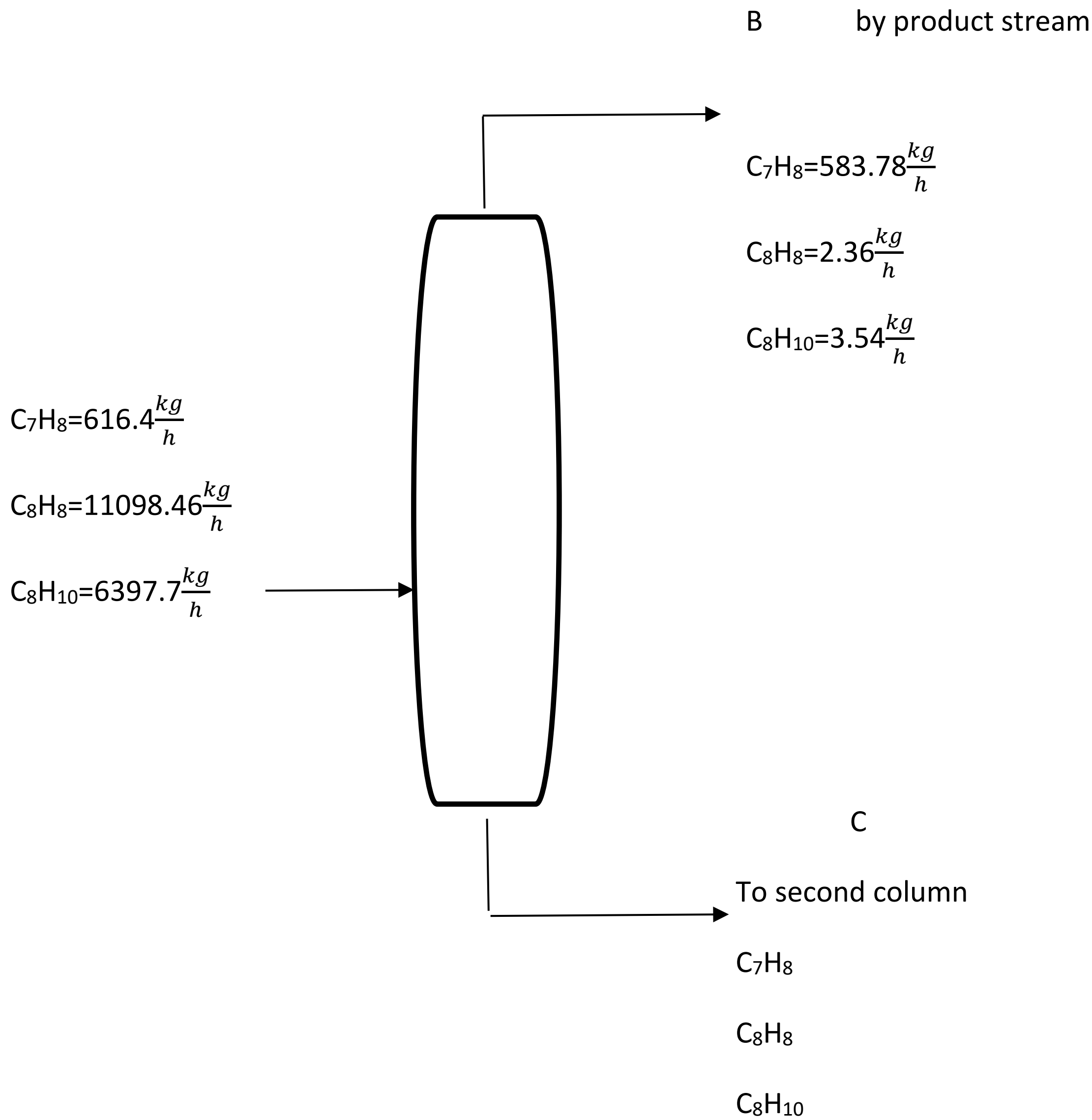
$W = W_1 + V$

$V = W - W_1$

$V = 27935.28 - 27851.474$

$V = 83.81 \frac{kg}{h}$

3.5 Material balance on first column:



To determine flow rates in stream C

$C_7H_8 = 616.4 - 583.78 = 32.62\frac{kg}{h}$

$C_8H_8 = 11098.46 - 2.36 = 11096.1\frac{kg}{h}$

$C_8H_{10} = 6397.7 - 3.54 = 6394.16\frac{kg}{h}$

3.6 Material balance on Second Column:

All of them are calculated

R

$R = 6405.78\frac{kg}{h}$

$0.5\% C_7H_8 = 32.03\frac{kg}{h}$

$98\% C_8H_{10} = 6277.66\frac{kg}{h}$

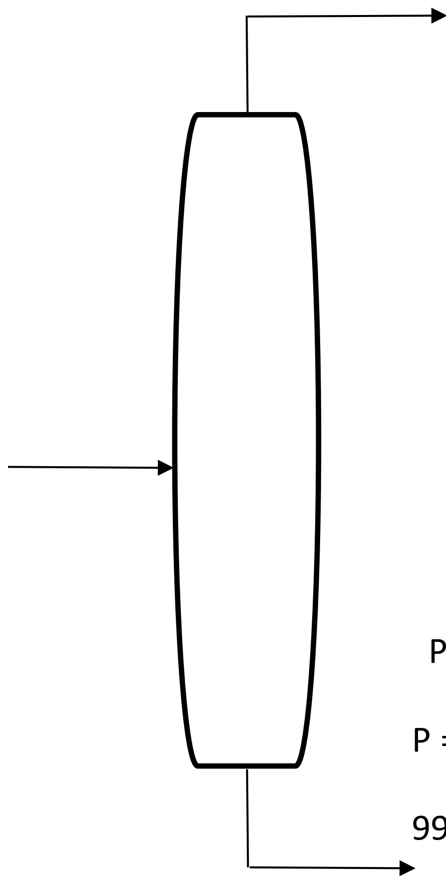
$1.5\% C_8H_8 = 96.1\frac{kg}{h}$

F

$C_7H_8 = 32.62\frac{kg}{h}$

$C_8H_8 = 11096.1\frac{kg}{h}$

$C_8H_{10} = 6394.16\frac{kg}{h}$



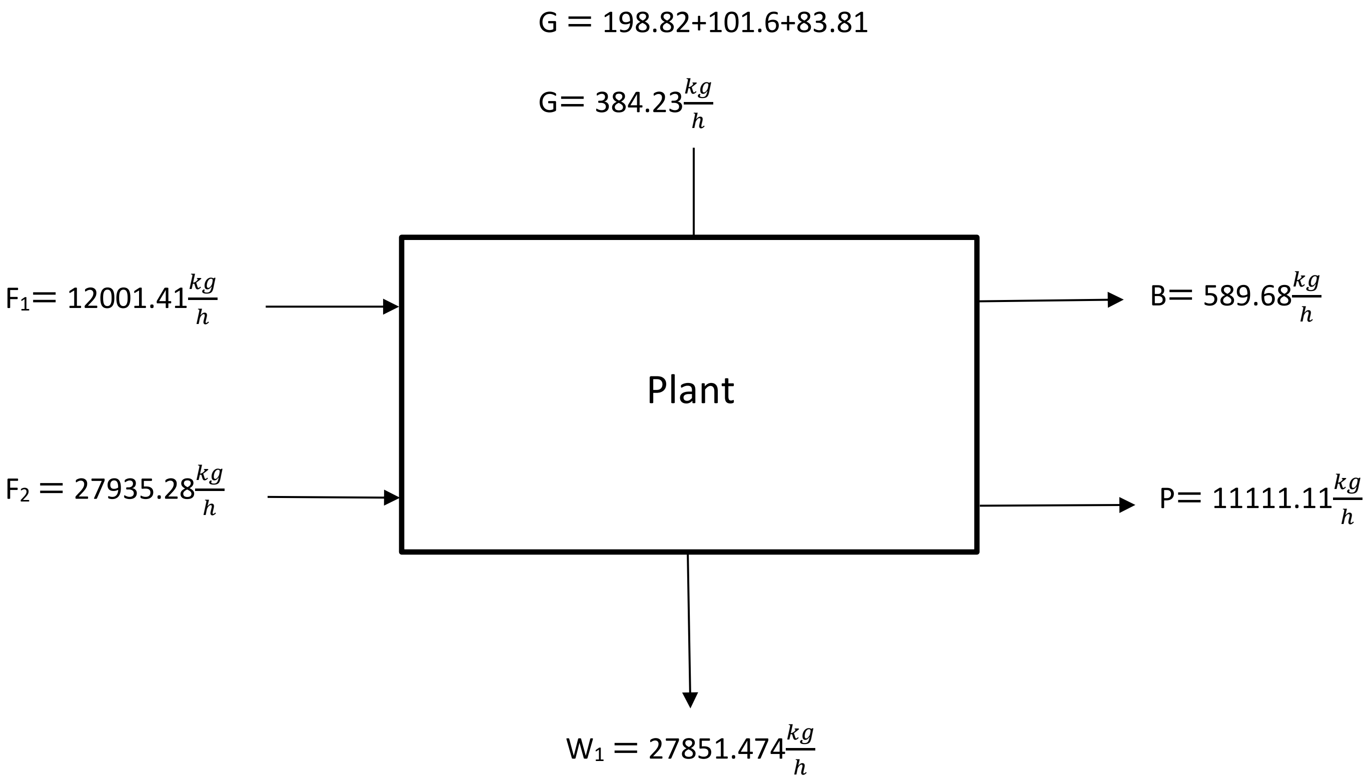
P

Product Stream

$P = 11111.11\frac{kg}{h}$

$99\% C_8H_8 = 10999.999$

$1\% C_8H_{10} = 111.1111$



Overall M.B

$F_1 + F_2 = G + W_1 + P + B$

$12001.41 + 27935.28 = 384.23 + 27851.474 + 11111.11 + 589.68 = 39936.6\,\frac{kg}{h}$

4 Chapter four: Energy balance

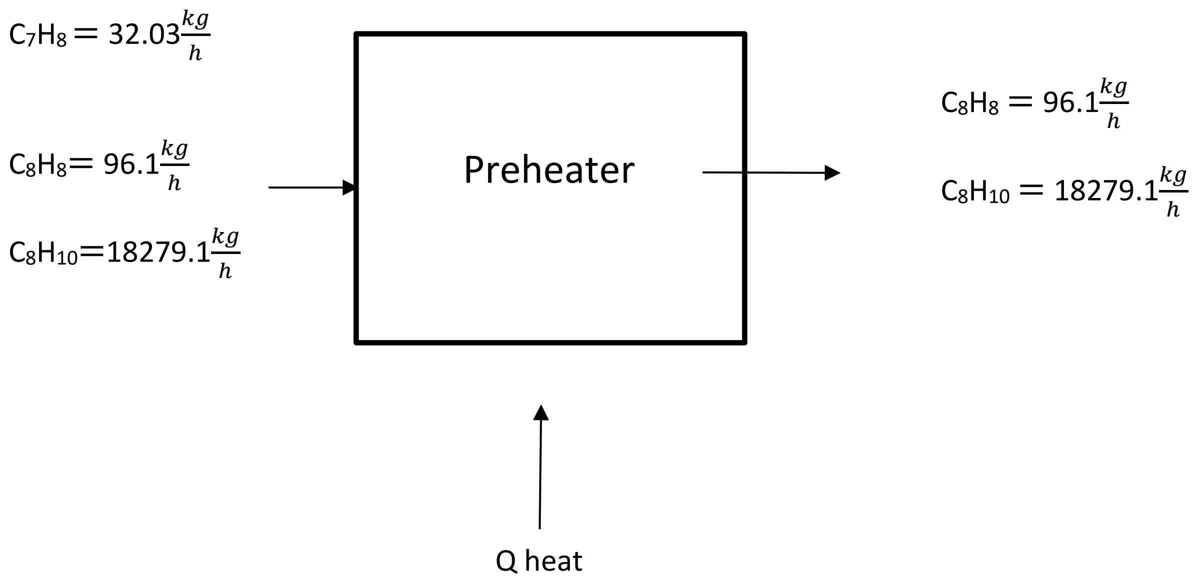
Gas heat capacity

$Cp = A+BT+CT^2+DT^3$ in $\frac{kJ}{kmol.k}$

Table 4-1 "Gas heat capacity coefficient"

Component	A	B	C	D
H_2	27,743	$9,273*10^{-3}$	$-1,380*10^{-5}$	$7,645*10^{-9}$
CH_4	19.251	$5.212*10^{-2}$	$1.197*10^{-5}$	$-1.131*10^{-8}$
H_2O	32.243	$1.923*10^{-3}$	$1.055*10^{-5}$	$-3.596*10^{-9}$
C_7H_8	-24.355	$5.124*10^{-1}$	$-2.765*10^{-4}$	$4.911*10^{-8}$
C_8H_{10}	-43.099	$7.071*10^{-1}$	$-4.810*10^{-4}$	$1.300*10^{-7}$
C_8H_8	-28.248	$6.158*10^{-1}$	$-4.023*10^{-4}$	$9.935*10^{-8}$

4.1 Energy balance on preheater:



This liquid is heated from 65.7℃ to bubble point and superheated to 225℃ [8]

By Antione equation $\ln P\ /Kpa = \mathrm{A} - \frac{B}{T+C}$ [9]

P=2atm

Table 4-2 "Antione equation constants"

Components	A	B	C
EB	14.0045	3279.47	−59.95
C_7H_8	14.0098	3103.01	−53.36
C_8H_8	14.3114	3505.78	−53.21

Table 4-3"Boiling point at 2 atm "

Components	T_{boil}
C_7H_8	134℃
C_8H_8	175 ℃
C_8H_{10}	164℃

At this pressure bubble point = boiling point of EB

$$Q_{heat} = \sum \mathrm{ni}\, C_{p\;liq}\,(T_{in} - T_{boil}) + \sum \mathrm{mi}\,\lambda + \sum \mathrm{ni} \int_{T_{boil}}^{498} C_{p\;gas}\, dT$$

$$C_{Pavg} = \frac{1}{\Delta T} \cdot \int_{T1}^{T2} C_{p\;liq}\, dT$$

Table 4-4"Liquid heat capacity coefficient"

Components	A	B	C	D
EB	102.11	55959×10^{-1}	-1.5609×10^{-3}	2.0149×10^{-6}
C_8H_8	66.737	8.405×10^{-1}	-2.1615×10^{-3}	2.3324×10^{-6}
C_7H_8	83.703	5.1666×10^{-1}	-1.4910×10^{-3}	1.9725×10^{-6}

Table 4-5"heat capacity at (T1 - Tboil)"

components	Cp_{avg} $in\ \frac{kJ}{kg.k}$
C_7H_8	1.91
C_8H_8	1.97
C_8H_{10}	1.99

$\lambda_i = A(1 - \frac{T}{TC})^{n}$ in $\frac{kJ}{mol}$

λ_i = Enthalpy of vaporization, kJ/mol

Table 4-6"Enthalpy of vaporization coefficient"

components	A	T	T_c	n
C_7H_8	50.139	407	591.79	0.383
C_8H_8	65.327	448	648	0.558
C_8H_{10}	54.788	437	617.17	0.388

Table 4-7"vaporization enthalpy values at boiling point"

components	$\lambda i\ in\ \frac{kJ}{Kg}$
C_7H_8	326.1
C_8H_8	335.9
C_8H_{10}	320.56

Q_{heat} = 3474551.12+5902273.3+2070506.83

$Q_{heat} = 11447331.25\frac{kJ}{h}$

This heat is supplied by saturated steam at 260°C and 4692 Kpa at these conditions $\lambda = 1662.5\frac{kJ}{kg}$

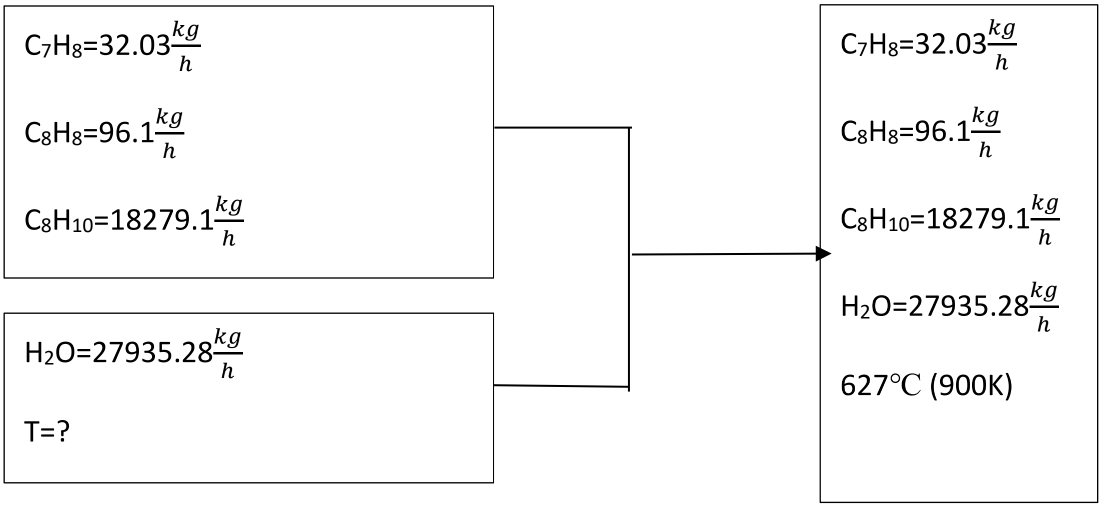
$Q = m\,\lambda$

$m = \frac{11447331.25}{1662.5}$

$m = 6885.6\frac{kg}{h}$

4.2 Energy balance on mixing point

EB at 225°C is mixed with steam[7]



$Q_{in} = Q_{out}$

$Q_{in} = \sum n_i \int_{T_{ref}}^{498} Cpi\ dT + n_{H20}\int_{T_{ref}}^{T} C_{pH_2o} dT$

Table 4-8"calculation of Cp integration from Tref -498 K"

Component	$n_i\int_{298}^{498} C_{pi}\ dT\ \ \frac{kJ}{h}$
C_7H8	9670.6
C_8H_8	29278.3
C_8H_{10}	5836899.94
H_2O	$1551.96 \int_{298}^{T} C_{pH_2o}\ dT$

$\sum n_i \int_{298}^{498} Cpi\ dT = 5875848.84\frac{kJ}{h}$

$Q_{out} = \sum ni \int_{T_{ref}}^{900} Cpi\ dT$

Table 4-9 "calculation of Cp integration from Tref -900 K"

Component	$ni\int_{298}^{900} Cpi\ dt$
C_7H8	$39660.9\ \frac{kJ}{h}$
C_8H_8	$117293.33\frac{kJ}{h}$
C_8H_{10}	$23703740.4\frac{kJ}{h}$
H_2O	$34130052.5\frac{kJ}{h}$

$Q_{out}= 57990747.13\frac{kJ}{h}$

$1551.96\int_{298}^{T} C_{pH_2o}\ dT\ =57990747.13- 5875848.84$

$\int_{298}^{T} Cp\ dt = 33580$

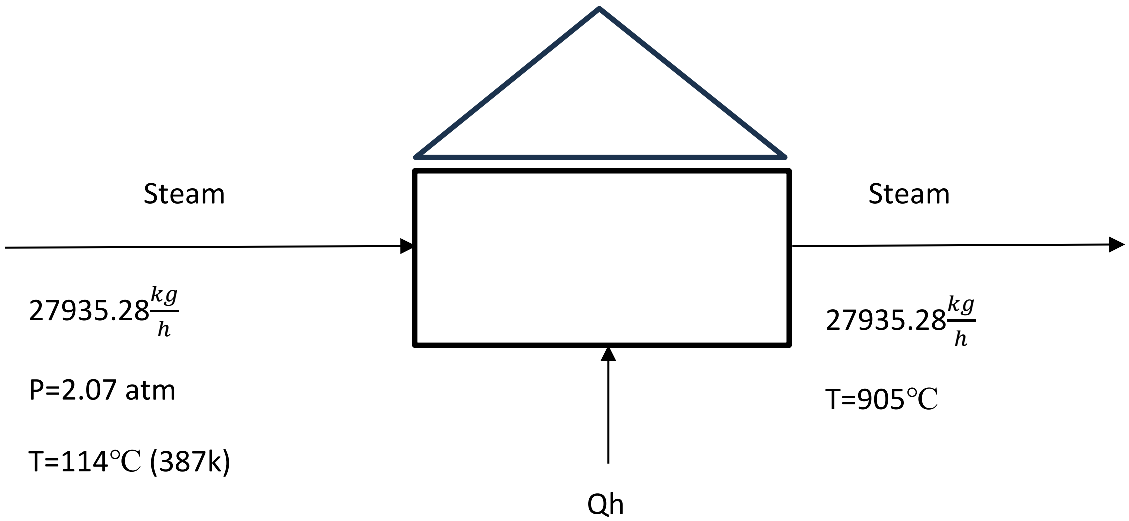
$(32.243)(T\text{-}298)+ \frac{1.923\times10^{-3}}{2}(T^2-298^2) + \frac{1.055\times10^{-5}}{3}$

$(T^3-298^3)+ \frac{-3.596\times10^{-9}}{4}\ (T^4-298^4) = 33580$

By mat lab

Steam temp=1178k=905°C

4.3 Energy balance on Furnace [7]



$\mathrm{Q_{in}} + \mathrm{Q_{heat}} = \mathrm{Q_{out}}$

$\mathrm{Q_{in}} = n_{steam} \int_{298}^{387} Cp\, dT$

$\mathrm{Qin} = 4696092.84\frac{kJ}{h}$

$Q_{out} = n_{steam} \int_{298}^{1178} Cp\, dt$

We calculated $\int_{298}^{1178} Cp\, dt = 33580$

$Q_{out} = n_{steam} \times 33580$

$Q_{out} = 1551.96 \times 33580$

$Q_{out} = 52114816.8\frac{kJ}{h}$

$Q_{heating} = Q_{out} - Q_{in}$

$Q_{heating} = 52114816.8 - 4696092.84$

$Q_{heating} = 47418723.96\frac{kJ}{h}$

4.4 Energy balance on reactor:

$Q_{in} + Q_{heating} = Q_{out} + Q_{reaction}$

$Q_{in} = \sum ni \int_{298}^{900} Cpi\ dT$

$Q_{in} = n_{C7H8}\int_{298}^{900} Cp\ dt + n_{C8H8}\int_{298}^{900} Cp\ dt + n_{C8H10}$

$\int_{298}^{900} Cp\ dt\ + n_{H20}\int_{298}^{900} Cp\ dt$

$Q_{in} = 57991653 \frac{kJ}{h}$

Table 4-10"formation heat"[10]

Components	ΔH at 298k in kJ/mol
C_8H_{10}	29.79
CH_4	-74.85
C_8H_8	147.36
C_7H_8	50
H_2O	-241.82
H_2	0

$$Q_{out} = \sum \text{ni} \int_{298}^{900} Cpi\ dT$$

Table 4-11"calculation of Cp integration from Tref -890 K"

Compo	Ni	$\int_{298}^{890} Cpi\ dt$	$\text{ni}\int_{298}^{890} Cpi\ dt$
CH_4	6.35	30680	194818
C_7H_8	6.7	110837.2	742609
C_8H_8	106.715	124222.2	13256369
C_8H_{10}	60.36	134483.582	8117429
H_2O	1551.96	21593.2	33511803
H_2	99.41	17392.5	1728984

$$Q_{out} = \sum \text{ni} \int_{298}^{900} Cpi\ dT$$

$$Q_{out} = 57552012 \frac{kJ}{h}$$

$$Q_{reaction} = \text{n1}\Delta Hr1(890k) + \text{n2}\Delta Hr2(890k)$$

$$\Delta Hr1(890) = \Delta Hr1(298) + \int_{298}^{890} \Delta Cp\ dt$$

From main reaction $\longrightarrow C_8H_{10} \rightleftarrows C_8H_8 + H_2$

$$\Delta Hr1(298K) = \sum_{\text{products}} \Delta H_f\ (298) - \sum_{\text{reactants}} \Delta H_f\ (298)$$

$$\Delta Hr1(298) = (\Delta H_{fC8H8} + \Delta H_{fH2}) - (\Delta H_{fC8H10})$$

$$\Delta Hr1(298) = (147.36+0) - (29.79)$$

$\Delta Hr1(298) = 117.57\frac{kJ}{mol} = 117570\frac{kJ}{kmol}$

$\int_{298}^{890} \Delta Cp\ dt = \int_{298}^{890} Cp\ H2 + \int_{298}^{890} Cp\ C8H8 - \int_{298}^{890} Cp\ C8H10$

$\int_{298}^{890} \Delta Cp\ dt = 17392.5 + 124222.2 - 134483.582$

$\int_{298}^{890} \Delta Cp\ dt = 7131\frac{kJ}{kmol}$

Now $\Delta Hr1(890) = 117570 + 7131$

$\Delta Hr1(890) = 124701\frac{kJ}{kmol}$

n1= $\frac{F1X1}{106}$ from M. B. calculated equ.(6)

$n_1 = \frac{11213.944\frac{kg}{h}}{106} = 105.8\frac{kmol}{h}$

Now from side reaction

$C_8H_2O + H_2 \longrightarrow C_7H_8 + CH_4$

$\Delta Hr2(298) = \sum \Delta H_{f(products)} - \sum \Delta H_{f(reactants)}$

$\Delta Hr2(298) = (50 + (-74.85)) - (29.79 + 0)$

$\Delta Hr2(298) = -54.64\frac{kJ}{mol} = -54640\frac{kJ}{kmol}$

$\int_{298}^{890} \Delta Cp\ dT = \int_{298}^{890} Cp\ C8H10 + \int_{298}^{890} Cp\ CH4\ dT - \int_{298}^{890} Cp\ C8H10\ dT - \int_{298}^{890} Cp\ H2\ dT$

$\int_{298}^{890} \Delta Cp\ dT = (110837.2 + 30680 - 134483.582 - 17392.5)$

$\int_{298}^{890} \Delta Cp\ dT = -10359\ \frac{kJ}{kmol}$

Now $\Delta Hr2(890)\ =\ \Delta Hr2(298) + \int_{298}^{890} \Delta Cp\ dT$

$\Delta Hr2 =\ -54640 - 10359$

$\Delta Hr2(890) = -64999 \frac{kJ}{kmol}$

$n2 = \frac{F1X1}{106}$ also calculated from M.B

$n2 = \frac{672.82}{106} = 6.35 \frac{kmol}{h}$

$Q_{reaction} = n1 \Delta Hr(890) + n2\ \Delta Hr2(890)$

$Q_r = 12780622 \frac{kJ}{h}$

$Q_h = Q_{out} + Qr - Q_{in}$

$Q_h = (57552012) + (12780622) - (57991653)$

$Q_{heating} = 12340981 \frac{kJ}{h}$

4.5 Energy balance on first cooler

$Q_{\ removed} = Q_{out} + Q_{in}$

Q $_{\text{removed}} = \sum \text{ni} \int_{298}^{890} C_{p\ gas}\, dT - \sum \text{ni} \int_{298}^{549.75} C_{p\ gas}\, dT$

Table 4-12"calculation of Cp integration from Tref -549.75 K"

Compo.	Ni	$\int_{298}^{549.75} C_{pi\ gas}\, dT$ in $\frac{KJ}{kmol}$
C_7H_8	6.7	36696
C_8H_8	106.715	41942
C_8H_{10}	60.36	44920
CH_4	6.35	10729
H_2O	1551.96	8739
H_2	99.41	7340

Q$_{\text{removed}} = \sum \text{ni} \int_{298}^{890} C_{p\ gas}\, dT\ (calculated) + \sum \text{ni} \int_{298}^{549.75} C_{p\ gas}\, dT$

$Q_{removed}\ = 57552012 - 21793459 = 35758553\ \frac{KJ}{h}$

4.6 Energy balance on second cooler:

$$Q_{removed} = Q_{in} - Q_{out}$$

$$Q_{\text{ removed}} = \sum \text{ni} \int_{298}^{549.75} C_{p\ gas}\, dT - \sum \text{ni} \int_{298}^{419.75} C_{p\ gas}\, dT$$

Table 4-13 "calculation of Cp integration from Tref -419.75 K"

Compo.	ni	$\int_{298}^{419.75} C_{pi\ gas}\, dT$ in $\frac{KJ}{kmol}$
C_7H_8	6.7	15330
C_8H_8	106.715	17673
C_8H_{10}	60.36	18786
CH_4	6.35	4745
H_2O	1551.96	4155
H_2	99.41	3536

$$Q_{removed} = 21793459 - 9952646 = 11840813 \frac{KJ}{h}$$

4.7 Energy balance on third cooler:

$$Q_{\text{removed}} = \sum \text{ni} \int_{419.75}^{T_{boil}} C_{p\,gas}\, d \; + \sum \text{mi}\, \lambda + \sum \text{ni}\, C_{p\,liq}\, (T_{out} - T_{boil})$$

by Antoine equation.

Table 4-14"Boiling point at 1.65 atm"

Component	T_{boil} at 1.65atm
C_7H_8	129℃
C_8H_8	159℃
C_8H_{10}	154℃
H_2O	110℃

Table 4-15"calculation of Cp integration"

Comp- that condensed	ni	$\int_{419.75}^{T_{boil}} C_{pi\,gas}\, dT$ in $\frac{KJ}{kmol}$	$\int_{419.75}^{344.5} C_{pi\,gas}\, dT$ in $\frac{KJ}{kmol}$ for comp. that not condensed
C_7H_8	6.7	-2536.5	
C_8H_8	106.715	2066.7	
C_8H_{10}	60.36	1304.4	
H_2O	1551.96	-1267.24	
H_2	99.41	------------------	-2189.44
CH_4	6.35	------------------	-3031

Table 4-16"vaporization enthalpy values at boiling point"

Component	λi at T_{boil} in $\frac{kJ}{kg}$
C_7H_8	352.35
C_8H_8	340.27
C_8H_{10}	327.35
H_2O	2168.94

$\sum mi\ \lambda = 66677789 \frac{kJ}{h}$

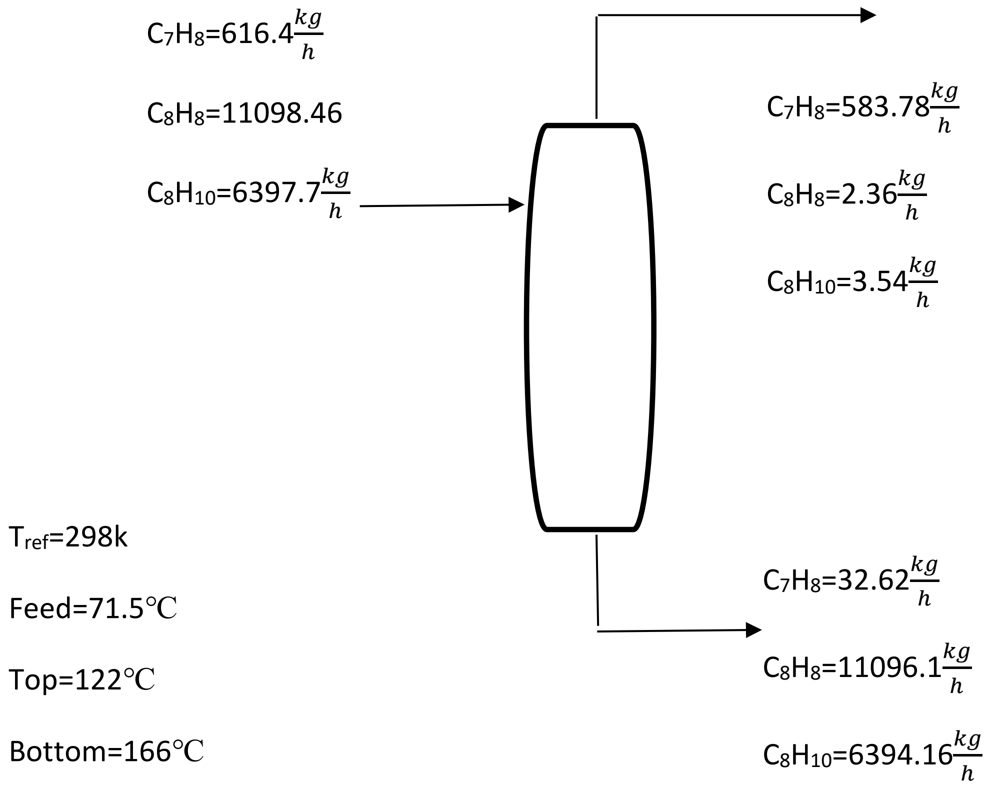
Table 4-17"liquid(Cp)avg"

Component	Cp avg Liquid in $\frac{kJ}{kg}$
C_7H_8	171.6
C_8H_8	204.1
C_8H_{10}	201.8
H_2O	75.4

$\sum ni\ C_{p\ avg.liq}\ .(T_{out} - T_{boil}) = -7481994$

$Q_{removed} = -1921318 + 66677789 - 7481994 = 9765838\ \frac{kJ}{h}$

4.8 Energy balance on first tower:



We have to calculate $C_{p\ avg}$ of all 3 components from T_{ref} to T_{stream} By Using Ludwig's data.

Table 4-18"liquid (Cp)avg at Tref - stream temp."

Components	C_{pavg} 25−71.5 ℃	C_{pavg} 25−122 ℃	C_{pavg} 25−166 ℃
C_7H_8	1.75	1.81	1.864
C_8H_8	1.84	1.88	1.93
C_8H_{10}	1.77	1.82	1.87

$Q_{in}=\sum C_{p\ avg}$ mi ΔT

Q_{in}= (616.4×1.75) + (11098.46×1.84) + (6397.7×1.77) (3445.5-298)

Q_{in}= 1526307 $\frac{KJ}{h}$

$Q_{\ out} = \sum C_{p\ avg}$ mi ΔT + $\sum C_{p\ avg}$ mi ΔT

$Q_{\ out} = \{(583.78 * 1.81)\ +\ (2.36 \times 1.88)\ +\ (3.54 \times 1.82)\ (395 - 298)\} + \{(32.62 \times 1.864)\ +\ (11096.1 \times 1.93)\ +\ (6394.16 \times 1.87)\ (439 - 298)\}$

Q_{out} =103550+4714103 = 4817653$\frac{KJ}{h}$

4.9 Energy on 2nd tower:

$C_7H_8 = 32.03 \frac{kg}{h}$

$C_8H_8 = 6277.66 \frac{kg}{h}$

$C_8H_{10} = 96.1 \frac{kg}{h}$

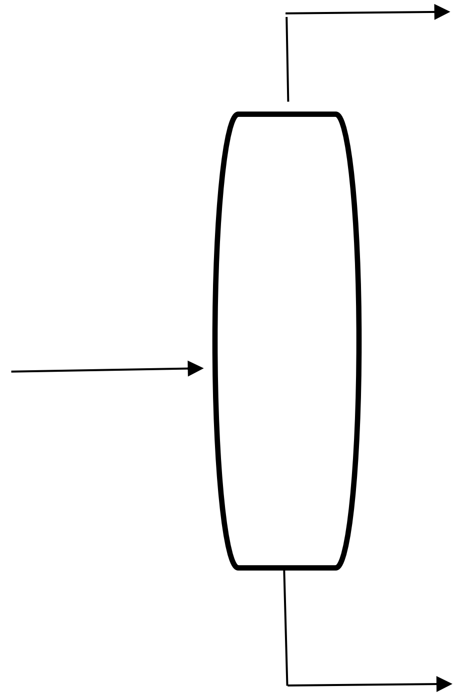
T= 142℃

$C_7H_8 = 32.03 \frac{kg}{h}$

$C_8H_8 = 11096.1 \frac{kg}{h}$

$C_8H_{10} = 6394.16 \frac{kg}{h}$

T = 166℃



$C_8H_8 = 10999.999 \frac{kg}{h}$

$C_8H_{10} = 111.1111 \frac{kg}{h}$

T = 175 ℃

Table 4-19"liquid (Cp)avg at Tref - stream temp."

Component	$C_p avg \frac{kJ}{kg.k}$ 25-166℃	$C_p avg \frac{kJ}{kg.k}$ 25-142℃	$C_p avg \frac{kJ}{kg.k}$ 25-175℃
C_7H_8	1.864	1.83	
C_8H_8	1.93	1.9	1.94
C_8H_{10}	1.87	1.84	1.88

$Q_{in} = \sum C_{p\ avg}$ mi ΔT

Q_{in}= (32.62×1.864)+(11096.1×1.93) + (6394.16×1.87)(439-298)

Q_{in}=4714103$\frac{kJ}{h}$

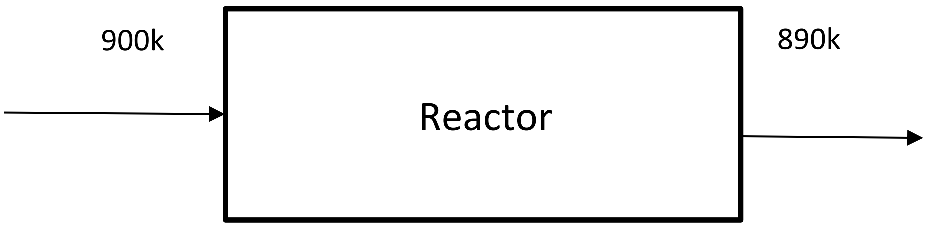
Q_{out}= $\sum C_{p\ avg}$ mi ΔT + $\sum C_{p\ avg}$ mi ΔT

$$[(32.03 \times 1.83)\ +\ (6277.66 \times 1.9)\ +\ (96.1 \times 1.84)(415 - 298)\ ] +$$
$$[(10999.999 \times 1.94)\ + (111.111 \times 1.88)(448 - 298)]$$

Q_{out} =1423070+3232333 $= 4655403\frac{kJ}{h}$

5 Chapter five: equipment design

5.1 reactor design



$C_7H_8 = 6.7 \frac{kmol}{h}$

$C_8H_8 = 106.715 \frac{kmol}{h}$

$C_8H_{10} = 60.36 \frac{kmol}{h}$

$H_2 = 99.41 \frac{kmol}{h}$

$CH_4 = 6.35 \frac{kmol}{h}$

$H_2O = 1551.96 \frac{kmol}{h}$

Total $=1831.48 \frac{kmol}{h}$

$P_i = P_t . \frac{Fi}{Ft}$

P_i=partial pressure

P_t=total pressure

Table 5-1"Reparametrized parameter estimates, standard deviations,95% confidence intervals for the Hougen-Watson kinetic model at all temperatures"

Parameter	unit	estimate
A_{EB}*	$\frac{1}{bar}$	9.648
A_{st}*	$\frac{1}{bar}$	34.93
A_{H2}*	$\frac{1}{bar}$	3.577
A1	$\frac{kmol}{kg.cat.hr}$	0.2539
A2	$\frac{kmol}{kg.cat.hr}$	0.02132
Ea1	$\frac{kJ}{mol}$	175.38
Ea2	$\frac{kJ}{mol}$	474.76
ΔHa,EB	$\frac{kJ}{mol}$	-102.22
ΔHa,ST	$\frac{kJ}{mol}$	-104.56
ΔHa,H_2	$\frac{kJ}{mol}$	-117.95

$P_{EB}=1.8.\frac{60.36}{1831.48} = 0.059atm$

$P_{st}=1.8.\frac{106.715}{1831.48}=0.1049atm$

$P_{H2}=1.8.\frac{99.41}{1831.48}=0.0977atm$

$Kj= Aj\ EXP\left[\frac{-\Delta H_{a,j}}{R}.(\frac{1}{T}+\frac{1}{Tr})\right]$

Kj = (Adsorption constant)

T_r = 893k

$K_{EB}=9.648\ EXP\left[-\frac{-102.22\times10^{3}\ \frac{J}{mol}}{8.314}.(\frac{1}{890}+\frac{1}{893})\right]$

K_{EB}=10.11 bar $^{-1}$

K_{st}=36.63 bar $^{-1}$

K_{H2}=3.77 bar $^{-1}$

$X_{EB} = \frac{F_{EB}-F_{EB^\circ}}{F_{EB}{}^\circ} = \frac{172.44-60.36}{172.44}=65\%$

$X_{TO}=\frac{F_{TO}-F_{TO^\circ}}{F_{EB^\circ}}=3.68\%$

$X_{H2}=\frac{F_{H2}-F_{H2^\circ}}{F_{EB^\circ}}= 57.6\%$

$X_{ST}=\frac{F_{ST}-F_{ST^\circ}}{F_{EB^\circ}}= 61.3\%$

$K_i = A_i\, e^{\left(\frac{-Eai}{R}\cdot\left(\frac{1}{T}-\frac{1}{Tr}\right)\right)}$

K_i = Constant rate

T=890

T_r =893

$K_1 = 0.2539\, e^{\left(-\frac{-175.38\times10^3 \frac{J}{mol}}{8.314}\cdot\left(\frac{1}{890}-\frac{1}{893}\right)\right)}$

$K_1 = 0.234\, \frac{\text{kmol}}{\text{kg.cat.hr}}$

$K_2 = 0.0172\, \frac{\text{kmol}}{\text{kg.cat.hr}}$

To calculate K_{eq} we have K_{eq} At 620°C =0.336 bar, so by van't Hoff

$\ln \frac{\text{Keq at 890}}{\text{Keq at 893}} = \frac{-\Delta Hr}{R}\ \left(\frac{1}{T} - \frac{1}{Tr}\right)$

ΔHr =124.83 $\frac{kJ}{mol}$

T_r =893k (620°C)

$\ln \frac{\text{Keq(890)}}{0.336} = \frac{-124.83*103}{8.314}\ \left(\frac{1}{890} - \frac{1}{893}\right)$

$\ln \frac{Keq}{0.336} = -0.0567$

$\frac{Keq}{o.336} = e^{-0.0567}$

Keq= 0.317 bar

$R_1 = \frac{K1\, K_{EB}(\, P_{EB} - \frac{P_{St}\, P_{H2}}{Keq})}{(1+K_{EB}\, P_{EB}+K_{H2}\, P_{H2}+K_{st}P_{st})^2}$

$R_2 = \frac{K1\ KEB\ PEB\ KH2\ PH2}{(1+K_{EB}\ P_{EB}+K_{H2}\ P_{H2}+K_{st}P_{st})^2}$

We have to convert partial pressure to bar

P_{EB}=0.059*1.01325=0.05978 bar

P_{st}=0.10629 bar

P_{H2}=0.09899 bar

$r_1=0.00182\ \frac{kmol}{kg_{cat}\ .hr}$

$r_2=1.125\times 10^{-4}\ \frac{kmol}{Kg_{cat}}$

$\rho_B=1422\ \frac{Kg_{cat}}{m^3}$

ρ_B = Bulk density

$W=F_{EB}°\int_0^X \frac{dx}{-rEB}$

$-r_{EB}=r_1+r_2 = 1.9325\times 10^{-3}\ \frac{kmol}{kg\ cat\ .hr}$

$W=172.44.\ (\frac{0.65}{1.9325\times 10^{-3}})$

W=58000 kg_{cat}

$V_{PBR}=\frac{W}{PB} = \frac{58000}{1422} = 40.8\ m^3$

$V_{PBR}=\frac{\pi}{4}D^2 L + \frac{\pi}{6}D^3$

$\frac{L}{D}$ = (2 -5), Let =3

L=3D

$V_{PBR} = \frac{\pi}{4} D^2 .3D + \frac{\pi}{6} D^3$

D = 2.42 m

L =7.26 m

To find thickness $t = \frac{PR}{SE-0.6P}$ +tc

P=Pfinl in psi = P_{in}+ 10% P_{in}

R = radius in inch

S= maximum allowable stress s from figer =180 bar =2611 P_{in}

E = joint efficiency = 0.9

T_c =corrosion allowance = 0.125 inch

P_{in} final =1.9 + (0.1) (1.9)× 14.696 = 30.7 Psi

$R = \frac{D}{2} \times 39.37 = 47.64$ inch

$t = \frac{(30.7)(47.64)}{(2611\times0.9)-(0.6\times30.7)}$ + 0.125= 0.75 inch = 19.1 mm = 2cm

Weight Hourly Space velocity

$WHsv = \frac{m_{EB}}{W_{cat}} = \frac{18278.6\,\frac{kg}{h}}{58000}$

WHsv = 0.315 $hour^{-1}$

Space time (T) = $\frac{1}{WHsr}$ = 3.2 hr

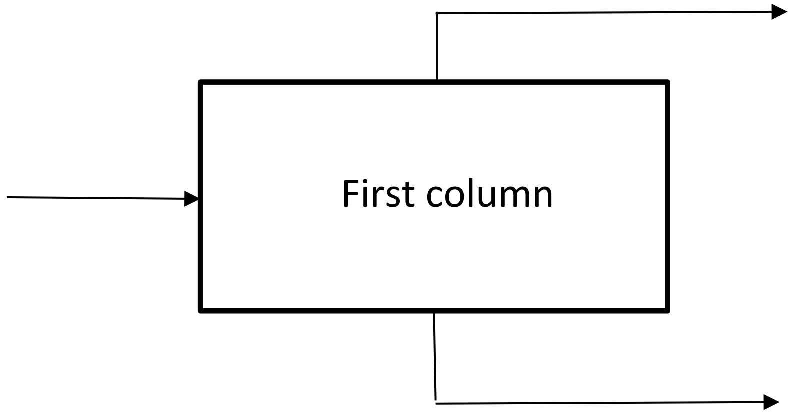
5.2 distillation design

F

C_7H_8=6.7 $\frac{kmol}{h}$

C_8H_8=106.715$\frac{kmol}{h}$

C_8H_{10}=60.35



D

C_7H_8= 6.35

C_8H_8=0,023$\frac{kmol}{h}$

C_8H_{10}=0,0333$\frac{kmol}{h}$

B

C_7H_8=0.355 $\frac{kmol}{h}$

C_8H_8=106.69 $\frac{kmol}{h}$

C_8H_{10}=60.32 $\frac{kmol}{h}$

Table 5-2"mole fractions"

Component	Mol% in F	Mol % Top	Mol % bottom
C_7H_8	0.039	0.99	2.12×10^{-3}
C_8H_8	0.614	3.6×10^{-3}	0.637
C_8H_{10}	0.35	5.2×10^{-3}	0.36

Light key has greatest mol % in top stream (LK= C_7H_8)

heavy key has greatest mol % in bottom stream (HK=C_8H_8)

First we have to find relative volatilities of (LK=A , HK =B)

α A = $\frac{KA}{KB}$, KA $\frac{PA°}{P}$, KB $\frac{PB°}{P}$

α A = $\frac{PA°}{PB°}$

$\ln Pi° = C_1 + \frac{C2}{T} + C_3 \ln T + C_4 T^{C5}$ in Pa [10]

Pi° = vapor pressure

Table 5-3"Vapor pressure coefficient"

Component	C_1	C_2	C_3	C_4	C_5
C_7H_8	76.945	-6729.8	-8.179	$5.3017*10^{-6}$	2
C_8H_8	105.93	-8685.9	-12.42	$7.5583*10^{-6}$	2

Table 5-4"Vapor pressure at stream temp."

Component	Pi at 71.5℃	Pi at 122 ℃	Pi at 166 ℃
C_7H_8	28.5 kpa	138 kpa	389 kpa
C_8H_8	8.56 kpa	52.2 kpa	168 kpa

Table 5-5"Relative volatility"

Component	αi at F	αi at D	αi at B
C_7H_8	3.3	2.64	2.32
C_8H_8	1	1	1

αi avg = $\sqrt[3]{\alpha f * \alpha\ top * \alpha\ bot}$

α LK avg = $\sqrt[3]{3.3 * 2.64 * 2.32}$

α LK avg = 2.72

α HK avg = 1

Calculation of minimum number of trays N_{min}

$$N_{min} = \frac{\ln(\left(\frac{XLK}{XHK}\right)D.\ \left(\frac{XHK}{XLK}\right)B)}{\ln(\alpha\ LK\ )avg}$$

$$N_{min} = \frac{\ln(\left(\frac{0.99}{3.6*10-3}\right).\ \left(\frac{0.637}{2.12*10-3}\right))}{\ln(2.72\ )}$$

N_{min} = 11

Minimum no . of trays is 11   Including reboiler

Calculation of minimum reflux ratio Rm

$$\frac{\alpha\ A\ .XAf}{\alpha\ A-\theta} + \frac{\alpha\ B\ .\ XBf}{\alpha\ B-\theta} = 1-q$$

q = 1 for saturated liquid

$$\frac{(2.72)(0.039)}{2.72-\theta} + \frac{(1)(0.614)}{1-\theta} = 0$$

θ = 2.4666 by mat lab

$$\frac{\alpha\ A\ .XAD}{\alpha\ A-\theta} + \frac{\alpha\ B\ \ XB\ .D}{\alpha\ B-\theta} = Rm+1$$

$$\frac{(2.72)(0.99)}{2.72-2.4666} + \frac{(1)(3.6*10-3)}{1-2.4666} = Rm+1$$

Rm = 9.6

Actual reflux ration

R = (1.2 → 1.5) Rm

R = 1.3× Rm = 12.5

Theoretical no of trays

$$\frac{Nth-Nmin}{Nth+1} = 0.75\ (1 - \frac{R-Rmin}{R+1})^{0.566}$$

$$\frac{Nth-Nmin}{Nth+1} = 0.75\ (1 - \frac{12.5-9.6}{12.5+1})^{0.566}$$

$$\frac{Nth-Nmin}{Nth+1} = 0.44$$

Nth = 20

$$\ln(\mu) = C_1 + \frac{C2}{T} + C_3 \ln T + C_4\, T^{C5} \quad \text{pa. s}$$

Table 5-6"Viscosity coefficient"

Component	C_1	C_2	C_3	C_4	C_5
C_7H_8	-226.08	6805.7	37.542	- 0.060853	1
C_8H_8	-22.675	1758	1.6701		
C_8H_{10}	-13.563	1208.6	0.377		

$$T_{avg} = \frac{T_{top}+T_{bott}}{2} = 144\ °C$$

Table 5-7"viscosity at avg temp."

Component	μ in pa. s /at T_{avg}
C_7H_8	1.77×10^{-4}
C_8H_8	2.29×10^{-4}
C_8H_{10}	5.55×10^{-1}

$(\mu)_{avg} = \sum \mu i \ Xi$

$= (1.77\times 10^{-4})\ (0.039) + (2.29 \times 10^{-4})\ (0.614) + (5.55\times 10^{-1})\ (0.35)$

$\mu_{avg} = 0.19$ pa. s = 190 mPa. s

Over all tray efficiency

$E° = 51 - 32.5\ (\ \log(\mu_{avg}\ .\ \alpha_{avg})\ )$

$E° = 51 - 32.5\ (\ \log(190 \times\ 2.72)\ )$

$E° = 50.2\ \%$

Actual no. of trays

$N_{act} = \frac{Nth}{E°} = \frac{20}{0.502}$

$N_{act} = 40$

Location of feed

$\log \frac{ND}{NB} = 0.206 \log \left[(\frac{B}{D}) \left(\frac{XHK\ f}{XLK\ f} * \frac{XLKB}{XHKD} \right)^2 \right]$

$\log \frac{ND}{NB} = 0.206 \log \left[(\frac{167.4}{6.41}) \left(\frac{0.614}{0.039} \times \frac{2.12\times10^{-3}}{3.6\times10^{-3}} \right)^2 \right]$

$\log \frac{ND}{NB} = 0.7$

$\frac{ND}{NB} = 10^{0.7}$

$\frac{ND}{NB} = 5$

ND = 5 NB

N_{act} = ND + NB = 40

40 = 5 NB + NB

NB = 6.6 =7

ND = 33

Number of plates above the feed tray = 33

number of plates below the feed Tray = 7

Table 5-8"Density coefficient"

Component	C_1	C_2	C_3	C_4
C_7H_8	0.8792	0.27136	591.75	0.29241
C_8H_8	0.7397	0.2603	636	0.300
C_8H_{10}	0.70041	0.26162	617.15	0.28454

$$\rho/\frac{mol}{dm3} = \frac{C1}{C2\ (1+\left(1-\frac{T}{C3}\right)^{C4}}$$

Table 5-9"Component's density"

Component	$\rho\frac{mol}{dm3}$ * MWi
C_7H_8	686.4 $\frac{kg}{m3}$
C_8H_8	713.4 $\frac{kg}{m3}$
C_8H_{10}	672 $\frac{kg}{m3}$

$(\rho_l)_{mix} = \sum(Xi\ Pi)$

$(\rho_l)_{mix} = 697.7\ \frac{kg}{m3}$

$\rho_v = \ \frac{P\ \times M_{avg}}{RT}$

$M_{avg} = \sum(Xi\ \times\ MWi\ )\ = 104.76\ \frac{Kg}{Kmol}$

$R = 0.0821\ \frac{atm\ .L}{mol\ .k}$

$\rho_v = \frac{(1.41)(104.76)}{(0.0821)(439)} = 4.1\ \frac{g}{L}$

$4.1 \times \frac{kg}{1000g} \times \frac{1000L}{m3} = 4.1\ \frac{kg}{m3}$

Typical plate spacing = 0.5 m

$V_f = (-0.171 \times Ps^2 + 0.27 \times Ps - 0.047)\ (\frac{\rho_l - \rho_v}{\rho_v})^{0.5}$

Ps = plate spacing

$Vf = (-0.171 \times (0.5)^2 + 0.27 \times 0.5 - 0.047)\ (\frac{697.7\ -4.1}{4.1})^{0.5}$

Vf = 0.6 m/s flooding velocity

V_w = maximum vapor flow rate $Ln = Rac \times D = 12.5 \times 6.41 = 80.125\frac{kmol}{hr}$

$Vn = Ln + D = 6.41 + 80.125 = 86.125\ \frac{kmol}{hr}$

$Vm = Vn = 86.54\ \frac{kmol}{hr}$ for liquid feed

$V_w = Vm + Vn = 173.08\ \frac{kmol}{hr}$

$V_w = \frac{173.08}{3600} * \text{Mavg} = 5\ \frac{kg}{s}$

$D = \sqrt{\frac{4\ VW}{\text{Pr}\ \pi\ Vf}} = \sqrt{\frac{(4)(5)}{4.1 * \pi * 0.6}}$

D = 1.6 m

Calculation of distillation high

Hc = (Nact – 1) * HS + ΔH + plate thicknes

Hs = Tray spacing = 0.5 m

ΔH = Liqiud hold up = 0.5 m

Plate thickness = 0.005 Nact

Hc = (40 – 1)(0.5) + 0.5 + 0.005 * 40

Hc = 20.2 m

Volume of column

$V = \frac{\pi}{4} D^2 * Hc = 40.6\ m^3$

Column- cross – section area

$Ac = \frac{\pi}{4} Dc^2 = 2\ m^2$

Net column area

$An = Ac * 0.85 = 1.7\ m^2$

Down comer area

$Ad = 0.15\ Ac = 0.3\ m^2$

Active area

$Aa = Ac - 2\ Ad = 1.4\ m^2$

Hole area

$Ah = 0.1\ Aa = 0.14\ m^2$

Weir length of tray

$\frac{Ad}{Ac} = 0.15$

$\frac{Lw}{dc}$ = 0.6 from figure 11.31 Coulson & Richardson 6th volume 3rd edition [11]

$Lw = 0.6 * 1.6 = 0.96\ m = 96cm$

$Lm = Vm + B = 293.91\frac{kmol}{h}$

$Lm = \frac{293.91 * Mavg}{3600} = 7.4\ \frac{kg}{s}$

$How = 750\ (\frac{Lm}{Lw * PL})^{0.66}$

Maximum weir liquid (how) = 37.2 mm

Minimum liquid rate = 70 % Lm = (0.7) (7.4) = 5.18 $\frac{kg}{h}$

Minimum (how) = $750\ (\frac{5.18}{(0.96)(697.7)})^{0.66}$

how = 29 mm

Take weir height (hw) = 50 mm

Hw+ how = 50 +29 = 79 mm liq

So, from fig 11.30 Coulson & Richardson 6th volume 3rd edition [11]

K_2 = 30.5

So, uh′ = $\frac{K2-0.9\ (25.4-D_h)}{\sqrt{\rho_v}}$

uh′ = $\frac{30.5\ -\ 0.9\ (25.4\ -\ 5)}{\sqrt{P4.1}}$

uh′ = 6 m/sec velocity through holes

Dry plate drop

$\frac{Ah}{Aa}$ = 0.1 so from fig 11.34 Coulson & Richardson 6th volume 3rd edition [11]

C_0 = 0.84

h_d = 51. $(\frac{\mathrm{uh}\prime}{\mathrm{C0}})^2 . \frac{\rho_v}{\rho_l}$

hd = 51. $(\frac{6}{0.84})^2 . \frac{4.1}{697.7}$

hd =15.3 mm liquid

Residual head

hr = $\frac{12.5*103}{PL}$ = 17.9 mm liquid

Total pressure drop

ht = hd + (h_w +h_{ow}) + hr

ht = 15.3 + (79) + 17.9

ht = 112.2 mm liquid

Total column pressure drop

dP = (9.81×10^{-3}) ht $\times \rho_l \times$ Nact = (9.81×10^{-3}) (112.2) (697.7) (40)

dP = 30.7 kpa

5.3 heat exchanger design

The heat exchanger which is used as cooler to cool the mixture of gases from reactor column from 276.6 to 146.6 by using steam, gases is corrosive and high temp.so it will be on tube side.

Operating Condition:

Temperature of a hot gases input $T_1 = 276.6$℃

Temperature of a cold gases output $T_2 = 146.6$ ℃

Temperature of a steam input $t_1 = 110$℃

Temperature of a steam output $t_2 = 180$ ℃

Step 1: Specifications: The specification is given:

46348 $\frac{Kg}{h}$ of gases is cooled by exchange with steam (single phase)

The gases pressure is 1.75 atm ,

water pressure is 2400 Kpa .

Fouling factors: gases is $5000 \frac{W}{m^2.℃}$, for steam is $8000 \frac{W}{m^2.℃}$

The mean temperature of gases $= \frac{276.6+146.6}{2} = 211.6$

The physical properties of gases at mean temperature:

$C_p = 1.981 \frac{KJ}{Kg.K}$

$\mu = 1.657 \times 10^{-4}\ (Pa.sec)$

$$\rho_{mix} = \frac{M_{(mix)avg} \times P}{RT}$$

Where:

$\rho_{mix}\ in\ \frac{Kg}{m^3}$

$M_{(mix)avg}\ in\ \frac{Kg}{Kmol}$

$P\ in\ Kpa$

R in $\frac{Kpa.m^3}{Kmol.K}$

T in (K)

$$\rho_{mix} = \frac{25.34 \times 177.32}{(8.314)(484.75)} = 1.2\ \frac{Kg}{m^3}$$

The mean temperature of steam $= \frac{110+180}{2} = 145℃$

The physical properties of steam at mean temperature:

$C_p = 1.9139 \frac{KJ}{Kg.K}$

$\mu = 139.7277 \times 10^{-6} (Pa. \sec)$

$$\rho = \frac{M \times P}{RT}$$

$$\rho = \frac{18 \times 2400}{(8.314)(418.15)} = 12 \ \frac{Kg}{m^3}$$

Energy balance on heat exchanger

$$Q_{gas} = Q_{steam}$$

$$\frac{46348}{3600} \times (1.981)(276.6 - 146.6) = m. (1.9139)(180 - 110)$$

$$m = 25 \ \frac{Kg}{s}$$

Heat duty $= 3349 \ Kw$

Step 2: Overall coefficient:

For exchanger of this type the overall coefficient will be take$600 \frac{W}{m^2 \ ℃}$

Step 3: Exchanger type and dimensions:

We use shell and tube heat exchanger, and start with one shell pass and two tube passes.

Mean temperature difference (ΔT_{lm}):

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln\left(\frac{T_1 - t_2}{T_2 - t_1}\right)}$$

$$\Delta T_{lm} = 61.82℃$$

$$R = \frac{T_1 - T_2}{t_2 - t_1} = 1.76$$

$$S = \frac{t_2 - t_1}{T_2 - t_1} = 0.41$$

From fig (Sinnott et al., 2005), $F = 0.76$

Step 4: Heat transfer area:

$$Q = U \times A \times \Delta T_{lm}$$

$$A = \frac{3349 \times 10^3}{(600)(47.57)} = 117m^2$$

Step 5: Layout and Tubs size:

Using split-ring floating head exchanger.

As the fluid is corrosive stainless steel is used.

Use 19 mm outside diameter, 15 mm inside diameter, 4.88 m long tube.

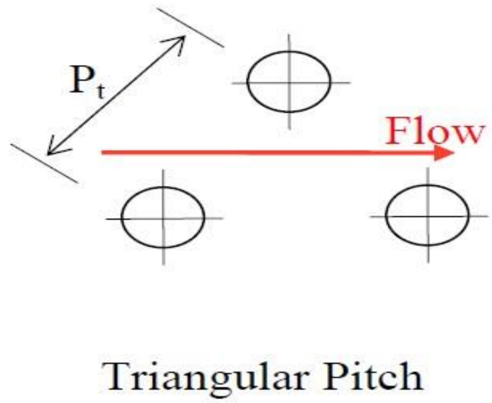


Figure 5-1"Triangular pitch"

$$l = 4.88 - \text{tube sheet thickness} = 4.88 - \times\, 0.025 = 4.83\ \text{m}$$

$$\text{Area of one tube} = \pi \times 19 \times 10^{-3} \times 4.83 = 0.2881\ m^2$$

$$\text{Number of tube } (N_t) = \frac{A}{A_t} = \frac{117}{0.2881} = 406$$

$$\text{So, for two pass, tubes per pass} = \frac{406}{2} = 203$$

$$\text{Tube cross} - \text{section area} = \frac{\pi}{4}\,(15 \times 10^{-3})^2 = 1.76625 \times 10^{-4}\text{m}^2$$

$$\text{Area per pass} = 203 \times 1.76625 \times 10^{-4} = 0.04\text{m}^2$$

$$\text{Volumetric flow} = \frac{\text{total mass flow}}{\rho} = \frac{46348}{(3600)(1.2)} = 10.7\,\frac{\text{m}^3}{\text{sec}}$$

$$\text{Tube side velocity } (\text{u}_\text{t}) = \frac{10.7}{0.04} = 268\ \frac{\text{m}}{\text{sec}}$$

Step 7: Bundle and shell diameter

For 2 pass ,$K_1 = 0.249$

$n_1 = 2.207$

$$D_b = d_0 (\frac{N_t}{K_1})^{(\frac{1}{n1})}$$

$$D_b = 19\left(\frac{406}{0.249}\right)^{(\frac{1}{2.207})} \qquad = 542 \text{ mm}$$

For a split – ring floating heat exchanger the typical shell clearance is 72 mm, so the shell inside diameter (Sinnott et al., 2005).

$D_s = D_b + clearance = 542 + 72 = 614\, mm$

Step 8: Tube side heat transfer coefficient:

$$R_e = \frac{\rho \times u \times d_i}{\mu_{mix}} = \frac{1.2 \times 268 \times 15 \times 10^{-3}}{1.657 \times 10^{-4}} = 29113$$

$$p_r = \frac{\mu_{mix} \times C_p}{K} = \frac{1.657 \times 10^{-4} \times 1.9581 \times 10^{3}}{0.03698} = 8.77$$

$$\frac{l}{d_i} = \frac{4.83}{15 \times 10^{-3}} = 322$$

$$j_h = 3.099 \times 10^{-3}$$

$$N_t = \frac{h_i \times d_i}{K_f} = j_h \times R_e \times P_r$$

$$h_i = 3.099 \times 10^{-3} \times 29113 \times 8.77^{0.33} \times \frac{0.03698}{15 \times 10^{-3}} = 455 \frac{W}{m^2 ℃}$$

This is clearly too low if U_0 is to be $600 \frac{W}{m^2 °C}$ the tube-side velocity did look low, so increase the number of tube passes to 4, This will halve the cross-sectional area in each pass and double velocity.

$$U_t = 2 \times 268 = 536 \frac{\mathrm{m}}{\mathrm{sec}}$$
$$R_e = 2 \times 29113 = 58226$$
$$j_h = 3.9 \times 10^{-3}$$
$$h_i = 3.9 \times 10^{-3} \times 58226 \times 8.77^{0.33} \times \frac{0.03698}{15 \times 10^{-3}} = 1146 \frac{\mathrm{W}}{\mathrm{m}^2 \cdot C^o}$$

Step 9: Shell side heat transfer coefficient:

For 4 passes, $k_1 = 0.175, n_1 = 2.285$

$$\mathrm{D_b} = 19 \times \left(\frac{1874}{0.175}\right)^{\left(\frac{1}{2.285}\right)} = 1102.33 \text{ mm}$$
$$\mathrm{D_s} = \mathrm{D_b} + \text{ Clearance } = 1102.33 + 74 = 1176.33 \text{ mm}$$
$$P_t = 1.25 \times d_o = 1.25 \times 19 = 23.75 \text{ mm}$$

$$A_S = \frac{P_t - d_o}{P_t} \times \mathrm{D_s} \times l_B$$

$$A_S = \frac{23.75 - 19}{23.75} \times 1176.33 \times 529.34 \times 10^{-6} = 0.1245 \text{ m}^2$$

Volumetric flow rate on shell side $= \frac{115}{12} = 9.5833 \frac{\text{m}^3}{\text{sec}}$

Shell side velocity $= \frac{9.5833}{0.1245} = 76.9 \frac{\text{m}}{\text{sec}}$

$$d_e = \frac{1.1}{d_o} \times (P_t^2 - 0.917 \times d_o^2) = \frac{1.1}{19} \times (23.75^2 - 0.917 \times 19^2)$$

$$d_e = 13.5 \text{ mm}$$

$$R_e = \frac{\rho \times u \times d_e}{\mu} = \frac{12 \times 76.9 \times 13.5 \times 10^{-3}}{139.7277 \times 10^{-6}} = 89157$$

$$j_h = 1.6 \times 10^{-3}$$

$$h_s = 1.601 \times 10^{-3} \times 89157 \times 9.28^{0.33} \times \frac{0.288}{13.5 \times 10^{-3}} = 6351.9 \frac{\text{W}}{\text{m}^2.\text{C}^o}$$

Step 10: Overall coefficients.

$$\frac{1}{U_o} = \frac{1}{h_s} + \frac{1}{h_{of}} + \frac{d_o \times \ln\left(\frac{d_o}{d_i}\right)}{2 \times k_w} + \frac{d_o}{d_i \times h_i} + \frac{d_o}{d_i \times h_{if}}$$

Where:

k_w = thermal conductivity of cupro - nickel alloy $= 50 \frac{W}{m \cdot C^o}$

$$\frac{1}{U_o} = \frac{1}{6351.9} + \frac{1}{8000} + \frac{0.019 \times \ln\left(\frac{19}{15}\right)}{2 \times 50} + \frac{19}{15 \times 1303} + \frac{19}{15 \times 5000}$$

$$U_o = 643.99 \frac{W}{m^2 \cdot C^o}$$

This is above the initial estimate of $600 \frac{W}{m^2 \cdot C^o}$ which may be acceptable.

Step 11: Pressure drop:

Tube side:

From fig. (Sinnott et al., 2005).

$$j_f = 3 * 10^{-3}$$

$$\Delta P_t = N_t \times \left[8 \times j_f \times \frac{l}{d_i} + 2.5\right] \times \frac{\rho \times u_t^2}{2}$$

$$\Delta P_t = 4 \times \left[8 \times 3 \times 10^{-3} \times \frac{4.83}{15 * 10^{-3}} + 2.5\right] \times \frac{11.084 * 66^2}{2} = 987.6\text{kP}$$

Shell side:

From fig. (Sinnott et al., 2005).

$$j_f = 2.3 \times 10^{-3}$$

$$\Delta P_s = 8 \times j_f \times \left(\frac{l}{l_B}\right) \times \left(\frac{D_s}{d_e}\right) \times \frac{\rho \times u_s^2}{2}$$

$$\Delta P_s = 8 \times 2.3 \times 10^{-3} \times \left(\frac{4.83}{529 \times 10^{-3}}\right) \times \left(\frac{1176.23}{13.5}\right) \times \frac{12 * 76.6^2}{2}$$

$= 5153.19$kp is not acceptable

Could be reduced by increasing the baffle pitch. Doubling the pitch halves the shell side velocity, which reduces the pressure drop by factor of approximately $\left(\frac{1}{2}\right)^2$.

$\Delta P_s = \frac{5153.19}{4} \times \frac{1}{2} = 323.07$kP(is acceptable)

This will reduce the shell side heat transfer coefficient by a factor of $\left(\frac{1}{2}\right)^{0.8}$ where ($h_o \propto u_s{}^{0.8}$)

$$h_s = 6351.9 \times (0.5)^{0.8} = 3648.2085 \frac{W}{m^2.C^o}$$

This gives an overall coefficient of $598.9925\frac{W}{m^2 \cdot C^o}$.

Step 12: Input and Output Nozzles:

Diameter of nozzle is given in equation below

$$\mathrm{D_m} = 293 \times m^{o0.53} \times \rho^{-0.37}$$

Nozzle for Input Hot gases

$$\mathrm{D_m} = 293 \times 60.55^{0.53} \times 11.084^{-0.37} = 1000\ \mathrm{mm} = 1\ \mathrm{m}$$

Nozzle for output steam

$$\mathrm{D_m} = 293 \times 115^{0.53} \times 12^{-0.37} = 1400\ \mathrm{mm} = 1.4\ \mathrm{m}$$

The vessel support used for the heat exchanger is two saddles.

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