MANUFACTURE OF HYDROGEN FROM NAPHTHA

EIGHT SEMESTER B.TECH PROJECT

Submitted in the partial fulfillment of

the Requirements for the Degree of

BACHELOR OF TECHNOLOGY

IN

CHEMICAL ENGINEERING

OF

ASSAM SCIENCE AND TECHNOLOGY UNIVERSITY

SUBMITTED BY

BEDANTA JYOTI DAS (19247)
DEBANGSHU KASHYAP (19249)
HIRAK JYOTI SARMA (19252)

DEPARTMENT OF CHEMICAL ENGINEERING
ASSAM ENGINEERING COLLEGE
JALUKBARI, GUWAHATI-781011

JUNE, 2023

CERTIFICATE OF SUBMISSION OF PROJECT

This is to certify that

BEDANTA JYOTI DAS, Roll No. 19247,

DEBANGSHU KASHYAP, Roll No. 19249,

HIRAK JYOTI SARMA, Roll No. 19252,

of B.Tech 8th Semester have jointly carried out the project entitled "PRODUCTION OF HYDROGEN FROM NAPHTHA" and submitted the report in partial fulfillment of the requirement for the Degree of Bachelor of Technology in Chemical Engineering of Assam Engineering College under Assam Science and Technology University, which may be accepted.

Dr. Bandana Chakraborty

Head of the Department

Department of Chemical Engineering

Assam Engineering College

Guwahati-13

ACKNOWLEDGEMENT

We are highly obliged to express our sincere and heartfelt gratitude to Miss. MOUSUMEE DAS, Department of Chemical Engineering, Assam Engineering College, Guwahati, for excellent guidance, constant encouragement, alert supervision and full cooperation throughout our project work.

Our sincere thanks and gratitude goes to Dr. Bandana Chakraborty, Head of the Chemical Engineering Department, for providing necessary facilities in carrying out our work.

Last but not the least we would like to convey our thanks to our friends and well-wishers whose helping hands, words of encouragement and criticism have always guided us towards the full completion of this work.

Name of Students: - Signatures:-

1. BEDANTA JYOTI DAS

2. DEBANGSHU KASHYAP

3. HIRAK JYOTI SARMA

CERTIFICATE OF COMPLETION

This is to certify that the following 8th semester B.Tech students of the department of Chemical Engineering of Assam Engineering College, Guwahati have successfully completed the project on “Production of Hydrogen from Naphtha” in partial fulfillment of the award of the degree of Bachelor of Technology(B.Tech) under Assam Science and Technology University.

Name of Students: -	Signatures:-
1. BEDANTA JYOTI DAS	
2. DEBANGSHU KASHYAP	
3. HIRAK JYOTI SARMA	

MISS MOUSUMEE DAS
Assistant Professor
Department of Chemical Engineering
Assam Engineering College
Guwahati-13

ABSTRACT

Our project “Production of Hydrogen from Naphtha” was such a theoretical project where we came across various industry equipments. We had to deal with various process variables like temperature, pressure in order to design equipments like heat exchangers and storage tanks from the modified material balance and energy balances of the individual units. This project helped us to understand the whole process of Production of Hydrogen from Naphtha, design, analysis and detailing of the various units involved in the process.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

SL.NO.	SYMBOL	DESCRIPTION	UNIT
1	A	Area of heat transfer	ft^2
2	C_P	Specific heat	Btu/lb °F
3	G	Mass velocity	lb/ft^2h
4	ID	Internal diameter	ft
5	m	Mass of component	kg
6	OD	Outer diameter	ft
7	P	Absolute Pressure	Psi or kgf/cm^2 or Kpa
8	Q	Amount of heat	KJ
9	T	Temperature	K or °F
10	T_O	Reference Temperature	K or °F
11	T_{avg}	Average Temperature of hot stream	K or °F
12	t_{avg}	Average Temperature of cold stream	K or °F
13	U	Heat Transfer co-efficient	Btu/hr ft^2 °F
14	U_C	Clean overall Heat transfer co-efficient	Btu/hr ft^2 °F
15	U_D	Overall Heat transfer co-efficient	Btu/hr ft^2 °F

PROJECT AT A GLANCE

TITLE: Production of Hydrogen from Naphtha

Process adopted: Steam reforming

Capacity of plant: 50000 MTPA

Naphtha input to process: 344.47 Kmol/hr

Steam input to process: 5267.706 Kmol/hr

Hydrogen output from the process: 3100.38 Kmol/hr

Overall material input to the process: 112133.32 Kg/hr

Overall material output from the process: 112133.32 Kg/hr

List of major equipments used in the plant:

1. Reformer
2. HT-Shift reactor
3. CO_2 Absorber
4. Pressure Swing Absorber
5. Steam Drum
6. Heat Exchanger
7. Cooler
8. Steam Superheater

Design of Equipments:

1. Shell and Tube Heat Exchanger

Shell	Tube
ID = 23 1/4	Number & length = 364, 8’0”
Baffle Spacing = 12 inch	OD= ¾ in, BWG = 16
Passes = 1	Passes = 2

2. Pressure Vessel and Head
   Vessel thickness = 5 mm (standard)
   Head thickness = 10 mm (standard)

CHAPTER 1

INTRODUCTION

This Chapter gives an insight of project. This project deals with the production of hydrogen from naptha. Hydrogen is the most abundant element in the universe. It is also the simplest consisting of one proton and one electron. However, since it is not found on Earth in is elemental form there are many different methods of producing it from hydrogen-containing molecules. Hydrogen is set to play an evermore important part of plans to decarbonise future global energy production and distribution. One of its important roles is as an energy vector, i.e., as a carrier of energy from a primary energy source to where that energy is needed. One major advantage is that when hydrogen is used as a fuel, for example in fuel cells, it is very clean. Water is the only product, and it is free from the emission of harmful pollutants produced in the combustion of hydrocarbon fuels, making it ideal for use in urban environments for heavy transport such as busses and for combined heat and power units in domestic and commercial buildings.

Hydrogen has another important role as a chemical feedstock, in fact the overwhelming current use of hydrogen is for its use in refineries, the production of ammonia for fertiliser and in the production of steel. The International Energy Agency (IEA) estimated that in 2018 the global hydrogen production amounted to 74 million tonnes. Currently hydrogen production is dominated (95%) by processes using natural gas (methane), resulting in the emission of 830 million tonnes of carbon dioxide (CO2) as a by-product.

Although hydrogen is abundant in the universe, free hydrogen is not readily found on Earth. Here it is found bound into molecules, the most abundant of which are water (H2O) and hydrocarbons, especially methane (CH4). To obtain free hydrogen these molecules must be split by providing energy, which can then later be recouped by a recombination with oxygen to produce water. Hence the description of hydrogen as an energy vector rather than a primary source of energy. The first, and by far the most universal method is by the steam reforming of natural gas, often known as Steam Methane Reformation (SMR). Here, steam and natural gas, treated to remove contaminants, are heated together at high pressure at ~ 900°C over a nickel-based catalyst. The result is a mixture of carbon monoxide (CO) and hydrogen known as syngas. Syngas is further treated in the water-gas shift reaction to produce more hydrogen and carbon dioxide. The CO2 produced is currently released into the atmosphere but can be used in as a by-product e.g. in food processing and packaging where, again, it is ultimately released into the atmosphere. The steam reforming process derives the heat necessary to drive the reaction from the combustion of natural gas producing more CO2.

Another route to providing the heat for the SMR reaction is by a process known as partial oxidation of methane, which evolves heat as the reaction takes place. The partial oxidation reaction can be coupled to the steam reforming reaction to make what is known as an autothermal reformer (ATR).

Pressure Swing Adsorbers (PSA)-

The PSAs are used to filter out remaining traces of carbon monoxide,carbon dioxide,and methane from the hydrogen.These leftover gases are used as fuel for the furnance,while the hydrogen is ready for the customers.

CHAPTER 2

LITERATURE REVIEW

In this chapter introduction of hydrogen, its history, its various properties, its importance and its sources are given. The various production technique for the production of hydrogen and a step analysis of the process is given with a brief comparison between them at the end, resulting in the selection of most feasible and economical process.

2.1 HYDROGEN-

Hydrogen is the chemical element with the symbol H and atomic number 1. Hydrogen is the lightest element. At standard conditions hydrogen is a gas of diatomic molecules having the formula H_2. It is colorless, odorless, tasteless, non-toxic, and highly combustible. Hydrogen is the most abundant chemical substance in the universe, constituting roughly 75% of all normal matter. Stars such as the Sun are mainly composed of hydrogen in the plasma state. Most of the hydrogen on Earth exists in molecular forms such as water and organic compounds. For the most common isotope of hydrogen each atom has one proton, one electron, and no neutrons.(1)

In the early universe, the formation of protons, the nuclei of hydrogen, occurred during the first second after the Big Bang. The emergence of neutral hydrogen atoms throughout the universe occurred about 370,000 years later during the recombination epoch, when the plasma had cooled enough for electrons to remain bound to protons.(5)

Hydrogen is nonmetallic (except it becomes metallic at extremely high pressures) and readily forms a single covalent bond with most nonmetallic elements, forming compounds such as water and nearly all organic compounds. Hydrogen plays a particularly important role in acid–base reactions because these reactions usually involve the exchange of protons between soluble molecules. In ionic compounds, hydrogen can take the form of a negative charge (i.e., anion) where it is known as a hydride, or as a positively charged (i.e., cation) species denoted by the symbol $H+$. The $H+$ cation is simply a proton (symbol p) but its behavior in aqueous solutions and in ionic compounds involves screening of its electric charge by nearby polar molecules or anions. Because hydrogen is the only neutral atom for which the Schrödinger equation can be solved analytically, the study of its energetics and chemical bonding has played a key role in the development of quantum mechanics.(3)

2.2 HISTORY OF HYDROGEN PRODUCTION-

Hydrogen gas was first artificially produced in the early 16th century by the reaction of acids on metals. In 1766–1781, Henry Cavendish was the first to recognize that hydrogen gas was a discrete substance, by naming the gas from a metal-acid reaction "inflammable air". He speculated that "inflammable air" was in fact identical to the hypothetical substance called "phlogiston" and further finding in 1781 that the gas produces water when burned. In 1783, Antoine Lavoisier gave the element the name hydrogen when he and Laplace reproduced Cavendish's finding that water is produced when hydrogen is burned.

Lavoisier produced hydrogen for his experiments on mass conservation by reacting a flux of steam with metallic iron through an incandescent iron tube heated in a fire. Anaerobic oxidation of iron by the protons of water at high temperature can be schematically represented by the set of following reactions:

1) $Fe + H_2O \rightarrow FeO + H_2$

2) $Fe + 3H_2O \rightarrow Fe_2O_3 + 3H_2$

3) $Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$

Hydrogen was liquefied for the first time by James Dewar in 1898 by using regenerative cooling and his invention, the vacuum flask. He produced solid hydrogen the next year. Deuterium was discovered in December 1931 by Harold Urey, and tritium was prepared in 1934 by Ernest Rutherford, Mark Oliphant, and Paul Harteck. Heavy water, which consists of deuterium in the place of regular hydrogen, was discovered by Urey's group in 1932. François Isaac de Rivaz built the first de Rivaz engine, an internal combustion engine powered by a mixture of hydrogen and oxygen in 1806. Edward Daniel Clarke invented the hydrogen gas blowpipe in 1819.(3)

2.3. PHYSICAL PROPERTIES OF HYDROGEN-

Table 2.1

Colour	Colourless
Taste	Tasteless
Odour	Odourless
Density	0.08988g/L(0°C, 1atm)
Relative vapour pressure	0.07
Melting point	-259.35°C
Boiling point	-252.88°C
Solubility in water	Slightly soluble
Bond dissociation energy	434kJ/mol
First I.P	1311 KJ.mol^{-1}
Speed of Sound(400K,1atm)	1518m/s

2.4 CHEMICAL PROPERTIES OF HYDROGEN-

The chemical properties of hydrogen depend mainly on its bond dissociation energy. Due to high bond dissociation energy (436 kJ/mol), high energy is required to break the H-H bond. This makes hydrogen quite stable and unreactive at ordinary temperature. Majority of the reactions of hydrogen takes place at a high temperature or in presence of ultraviolet radiation.(4)

Combustion:

Hydrogen is a combustible gas but is a non-supporter of combustion. When burnt, it burns with a pale blue flame in air or oxygen forming water. This reaction is highly exothermic (283kJ/mol)

$$2H_2 + O_2 \rightarrow 2H_2O$$

Reaction with metals:

At high temperatures, hydrogen reacts with strong electropositive metals like Na, K, Ca, etc. to produce metal hydrides.

$$H_2 + 2Na \rightarrow 2NaH$$

$$H_2 + Ca \rightarrow CaH_2$$

Reaction with non-metals:

Reaction with halogens:

The reactivity of hydrogen with halogens decreases with the decrease in the reactivity of the halogens. $F_2 > Cl_2 > Br_2 > I_2$

Hydrogen reacts with fluorine in dark at ordinary temperature to produce hydrogen fluoride.

$$H_2 + F_2 \rightarrow 2HF$$

In the presence of sunlight, hydrogen reacts with chlorine to produce hydrogen chloride.

$$H_2 + Cl_2 \rightarrow 2HCl$$

At about 4000C, hydrogen reacts with bromine to produce hydrogen bromide.

$$H_2 + Br_2 \rightarrow 2HBr$$

At about 4000C, in presence of Pt catalyst, hydrogen reacts with iodine to produce hydrogen iodide.

$$H_2 + I_2 \rightarrow 2HI$$

Reaction with nitrogen:

At 673K, at 200 atm pressure, in presence of Fe catalyst and Mo promoter, nitrogen reacts with hydrogen (1:3) to produce ammonia. This reaction is used to manufacture ammonia industrially by Haber's process.

$$N_2 + 3H_2 \rightarrow 2NH_3$$

Reaction with sulphur:

At 700K, when hydrogen gas is bubbled through molten sulfur, hydrogen sulfide gas is produced.

$$H_2 + S \rightarrow H_2S$$

Reaction with carbon:

Hydrogen reacts with carbon at 1275K to produce methane in the presence of Co or Ni catalyst.

$$2H_2 + C \rightarrow CH_4$$

At a further higher temperature (3300K), acetylene gas is produced.

$$2C + H_2 \rightarrow C_2H_2$$

Reduction of metal oxides and ions:

Hydrogen acts as a reducing agent. It can reduce oxides of some metals like Pb, Fe, Cu, Zn *etc*. to the corresponding metals.

$$CuO + H_2 \rightarrow Cu + H_2O$$

$$ZnO + H_2 \rightarrow Zn + H_2O$$

Reaction with carbon monoxide:

$$(CO + H_2) + H_2 \xrightarrow[300\text{-}400\ ^\circ\text{C},\ 300\ \text{atm}]{CuO + ZnO + Cr_2O_3} CH_3OH + \text{Heat}$$

2.5 USES OF HYDROGEN-

Hydrogen is used in the manufacture of ammonia by Haber's process.

In the manufacture of metal hydrides, HCl, methanol and vegetable ghee
In airships and weather balloons as a mixture of hydrogen and helium
In the manufacture of synthetic petrol by heating coal and heavy oils in the presence of the catalyst under high pressure.

Liquid hydrogen is used as rocket fuel in the space program.

In metallurgy, it is used as a reducing agent to obtain certain metals like Pb, Fe, Cu, Zn *etc.*from the respective metal oxide.

2.6 METHODS OF HYDROGEN PRODUCTION-

There are various types of process for hydrogen production—

Steam Reforming
Catalytic Partial Oxidation of Hydrocarbons
Coal Gasification

2.6.1 Steam Reforming-

Steam reforming of methane is a well-established industrial technique for hydrogen production. Carbon of one form or another has long been used to extract hydrogen from water. The oxygen contained in the steam causes oxidation of the fuel, resulting in hydrogen (H_2). Natural gas, but also methanol, light gasoline, biogas or biomass are primarily used as carbon-containing fuels or energy carriers. In this process, the water vapor required for the reaction can be added from the outside or can come from the respective feedstock itself.(1)

The chemical reaction of steam reforming is endothermic, which means that it consumes heat. It is often supported by a catalyst or the required heat is generated by the combustion of the fuel.

Conceivable sources of external heat include concentrated solar thermal energy, high-temperature nuclear reactors, or waste heat from internal combustion engines. Steam reforming yields a gas mixture whose energy content significantly exceeds that of the fuel used.

Functionality of steam reforming-

First, the long-chain hydrocarbons are split to form methane, hydrogen, carbon monoxide and carbon dioxide. The methane is then reacted with water at constant pressure and a temperature of between 800 and 900 degrees Celsius. To obtain pure hydrogen at the end, pressure swing adsorption systems or caustic absorption gas scrubbers are used. These filter out by-products such as carbon monoxide, carbon dioxide and methane down to a few thousandths.

When natural gas – whose main component is methane (CH4) – is used, the following reaction thus takes place during steam reforming:

$$CH_4 + H_2O \rightarrow CO + 3\ H_2$$

To increase the hydrogen yield in steam reforming, the resulting carbon monoxide can be converted to carbon dioxide and even more hydrogen by a second reaction. This procedure is called a water gas shift reaction:

$$CO + H_2O \rightarrow CO_2 + H_2$$

2.6.2 Catalytic Partial Oxidation of Hydrocarbons-

Hydrogen production from natural gas and heavier hydrocarbons is achieved by partial oxidation. A fuel-air or fuel-oxygen mixture is partially combusted, resulting in a hydrogen- and carbon monoxide-rich syngas. More hydrogen and carbon dioxide are then obtained from carbon monoxide (and water) via the water-gas shift reaction.Carbon dioxide can be co-fed to lower the hydrogen to carbon monoxide ratio.

The partial oxidation reaction occurs when a substoichiometric fuel-air mixture or fuel-oxygen is partially combusted in a reformer or partial oxidation reactor. A distinction is made between thermal partial oxidation (TPOX) and catalytic partial oxidation (CPOX). The chemical reaction takes the general form:

$$C_nH_m + n/2\ O_2 \rightarrow n\ CO + m/2\ H_2$$

2.6.3 Coal Gasification-

For the production of hydrogen from coal, coal gasification is used. The process of coal gasification uses steam and oxygen to break molecular bonds in coal and form a gaseous mixture of hydrogen and carbon monoxide. Carbon dioxide and pollutants may be more easily removed from gas obtained from coal gasification versus coal combustion. Another method for conversion is low-temperature and high-temperature coal carbonization.

CHAPTER 3

PROCESS SELECTION

From the table given below we have select steam reforming because it is most economical one

Table 3.1 : Comparison between different types of processes

Process	Steam Reforming	Catalytic Partial oxidation
Raw Material	Naphtha, heavy hydro carbon, natural gas	Naptha, heavy hydro carbon, natural gas
Purity of Product	99%	Produced syngas with H_2
Yield Conversion	65-75%	70%
Reaction	CnHm+nH2O→nCO+(n+m/2)H2	2CnHm+H2O+23/2O2→ nCO+nCO2+nCO2+(m+1)H2
Temperature	(700-1000)°C	1000°C and higher
Pressure	3-25 bar	40-100 bar
Catalyst	Nickel	Refractory supported Ni
Nature of reactor	Endothermic	Exothermic
Energy Requirement	206 KJ/mol	-38 KJ/mol

CHAPTER 4

PROCESS DESCRIPTION

In this chapter, process description of steam reforming hydrogen unit is given. The feed to the reformer furnace is comprised of feed containing Naphtha, mixed with recycle stream and Process steam, which enter Tubular reactor in which the reaction occurring. The reactions occurring in the reformer are steam-methane reforming reactions. The five reforming reactions occur mainly in the steam reformer while thermodynamics favour the shift reaction in the high-temperature shift converter.The feed is considered to be the desulphurized naptha. The desulfurized and dechlorinated hydrogen feed is mixed where the controlled reforming reactions changes the feed to methane. The conversion of carbon monoxide is strongly favoured by a low temperature and high steam quantity, but is independent of pressure. These reactions are suppressed by using excess of steam , mainly removing carbon as it is formed by a series of reactions. The conversion of methane with steam to CO and hydrogen is strongly favored by a high temperature low pressure and high steam ratios. In the shift convertors the carbon monoxide on reaction with steam gets converted to H_2 and CO_2. The unutilized steam is condensed in step cooling and then the reformed gas enters to PSA.The outlet composition is a function of both of temperature and equilibrium and catalyst activity.For the temperature Shift reaction the inlet temperature is 700K and the outlet temperature is 691 K. 60% conversion takes place in the HT shift reactor. PSA technology is used to purify reformed hydrogen rich feed gas and produce a product stream of very high purity hydrogen at pressure from the reformed gas and off gas impurities. The off gas stream is then sent to the steam reformer burner. This is mainly achieved in molecular sieves, which adsorb the contaminants and after pressurization the adsorber is again ready for reuse. The contaminats are collected at the surge drum which is located below at the bottom. The cyclic pressure variation occurring during the the surplus heat in the process gas at the reformer outlet is recovered (in E1) and used to generate super-heated steam. Part of this steam is mixed with feed, while the remainder is exported outside the unit. Every absorber operates repeated cyclic consisting of adsorption and regeneration phases without any change of temperature except that adsorption and desorption. The cyclic are staggered in order to provide a continous product and purge gas (tail gas) flow.. in the PSA the hydrogen is separated using molecular sieves which adsorb the contaminants and allow the hydrogen to pass with a process gas and once through recovery of 90%. To regenerate it it is necessary to depressurize to purge gas pressure which releases the contaminants and after pressurization the adsorber is reaThe shift reaction (equation13) occurring in the HT shift converter produces additional H2. The hot leaving the shift converter is used to preheat boiler feed water (in E2) and again it exchanges heat with in heat exchanger (E3), which is pass through the cooler in which temperature get dropped. Again output of heat exchanger (E3) goes as a input in CO2 Absorber where almost all CO2 is absorbed in CO2 Absorber, after that output is sent to pressure-swing Adsorption (PSA 1) where H2 Product is sent out, from this again the second stream is sent to pressure-swing Adsorption (PSA 2) where CO gas is received as output from second (PSA 2) another stream is sent to Heat exchanger (E4) from one stream exchanger heat with export stream and it is sent out as export stream out and another stream is mixed with recycled and sent out as purge. The PSA gas leaves at about 0.33kg/cm2. The product hydrogen is passed through a filter to remove any fines especially in the process of operation. A part of hydrogen is recycled through HRC. rest of the pure hydrogen is recovered through and sent to the battery under limit conditions .it is this pressure control which indirectly fixes the operating pressure of the reformer.rest of the pure hydrogen is sent to the battery limit under the conditions under a control pressure of 20kg/cm2.

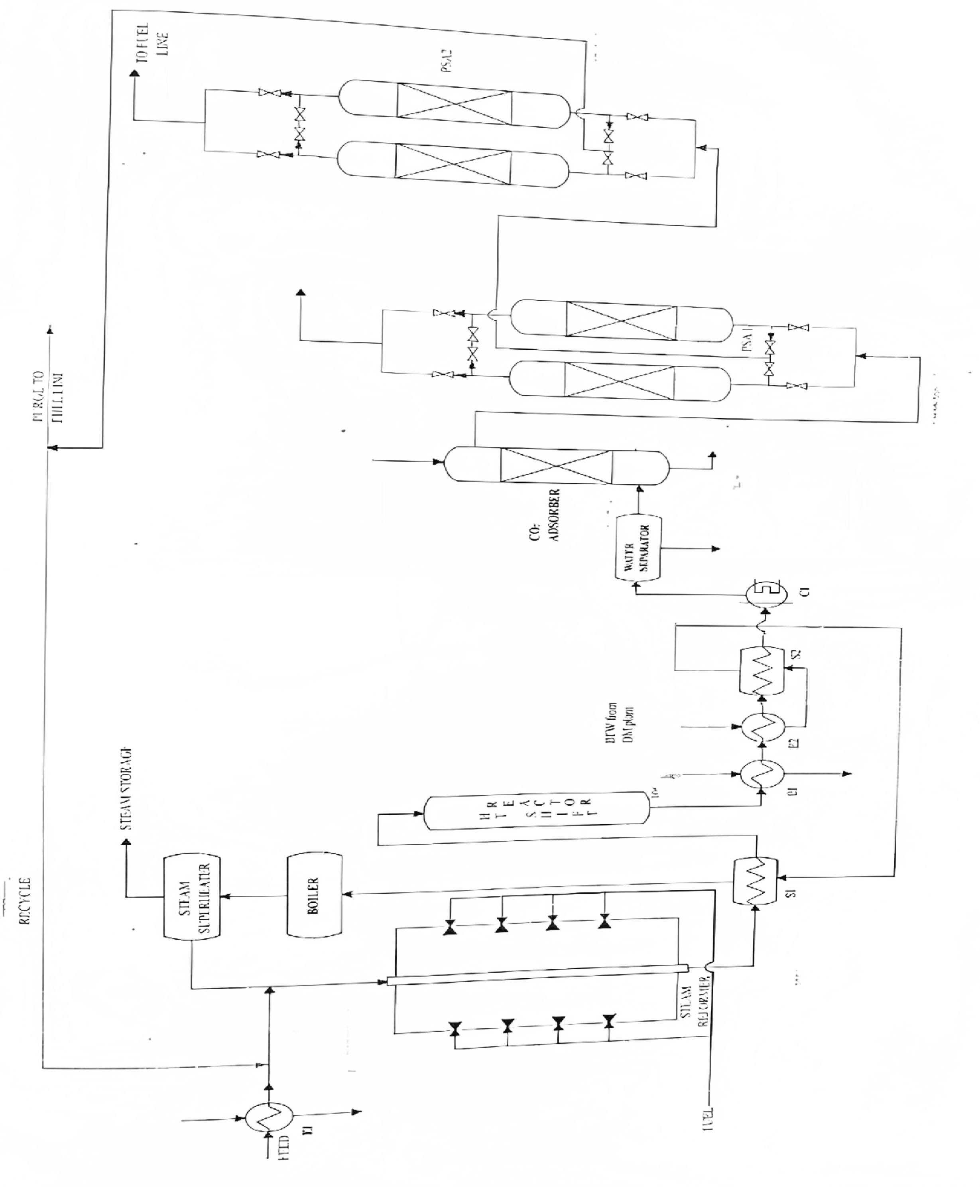


FIG 4.1 PROCESS FLOW DIAGRAM

CHAPTER 5

MATERIAL BALANCE

5.1 ASSUMPTION

1. Recycle stream mole fraction of N_2 should not exceed 10%

2. 65% of C_4H_{10}, C_5H_{12}, C_6H_{14} ,C_7H_{16} in reformer unit

3.55% conversion of CO to CO_2 in shift reactor

4.95% of absorption of CO_2 takes place in the C_{O2} absorber

5.2 INERT BALANCE

Recycle (mole fractions) R

X (C_4H_{10}) = x, X (C_5H_{12}) = 24x,

X (C_6H_{14}) = 16x, X (C_7H_{16}) = x, X (N_2) = 0.1

Purge (P)

X (C_4H_{10}) = x, X (C_5H_{12}) = 24x, X (C_6H_{14}) = 16x, X (C_7H_{16}) = x, X (N_2) = 0.1

Feed

C_4H_{10} = 2.26 kmol /hr

C_5H_{12} = 55.4 kmol /hr

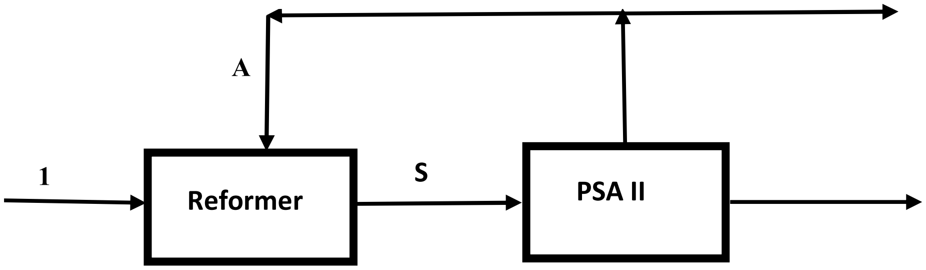
C_6H_{14} = 36.56 kmol /hr

C_7H_{16} =2.5 kmol /hr

Benzene= 3.18 kmol /hr

N_2 = 0.1 kmol /hr

Total = 100 kmol/hr



Let x, 24x, 16x and x be the mole fraction of the C_4H_{10}, C_5H_{12}, C_6H_{14} and C_7H_{16} in the purge and recycle stream & 0.1 is the mole fraction in the recycle stream.

So, x+24x+16x+x+0.1= 1

x=0.021

x_{C4H10}= 0.021

x_{C5H12}=0.514

x_{C6H14}=0.336

xC_7H_{16} = 0.021

By balancing N_2

0.1= 0.1* P

P= 1 kmol/hr

Assume in recycle= Butane: Pentane: Hexane: Heptane

1: 24 :16 :1

And 65% conversion of Butane, Pentane, Hexane and Heptane

A+1(Composition of the inlet stream to the reformer)

C_4H_{10}= 2.26+R*0.021

C_5H_{12}= 55.4+R*0.514

C_6H_{14}= 36.56+R*0.336

C_7H_{16}= 2.5+R*0.021

Composition of the outlet stream from the reformer

C_4H_{10}= 0.35(2.26+R*0.021)

C_5H_{12}= 0.35(55.4+R*0.514)

C_6H_{14}= 0.35(36.56+R*0.336)

C_7H_{16}= 0.35(2.5+R*0.021)

Component balance of C_4H_{10} at PSAII

0.35(2.26+R*0.021)= x(R+P)

=>0.35(2.26+R*0.021)= 0.021(R+1)

=>0.791+0.007R= 0.021R +0.021

=>0.014R= 0.769

=>**R=54.929**

Composition at purge stream

X (C_4H_{10}) = 0.021, X (C_5H_{12}) = 24x = 0.514, X (C_6H_{14}) = 16x=0.336, X (C_7H_{16}) = 0.021,

X (N_2) = 0.1.

5.3 MATERIAL BALANCE OVER THE REFORMER

Feed stream consists of

C_4H_{10} = 2.26 kmol/hr

C_5H_{12} = 55.4 kmol/hr

C_6H_{14} = 36.56 kmol/hr

C_7H_{16}= 2.5 kmol/hr

Benzene= 3.18 kmol/hr

N_2 = 0.1 kmol /hr

Total = 100 kmol/hr

Recycle stream consists of

Unconverted C_4H_{10} = (54.929)*(0.021) = 1.15 kmol/hr

Unconverted C_5H_{12} = (54.929*(0.514) = 28.23 kmol/hr

Unconverted C_6H_{14} = (54.929)*(0.336) = 18.45 kmol/hr

Unconverted C_7H_{16} = (54.929)*(0.021) = 1.15 kmol/hr

N_2 = 54.929 × 0.1 = 5.4929 kmol/hr

Mixed feed consist of

C_4H_{10} = (2.26+1.15) = 3.41 kmol/hr

C_5H_{12} = (55.4+28.23) = 83.63kmol/hr

C_6H_{14} = (36.56+18.45) = 55.01kmol/hr

C_7H_{16}= (2.5+1.15) = 3.65 kmol/hr

Benzene= 3.18 kmol/hr

N_2 = (0.1+5.4929) = 5.5929 kmol /hr

Now total amount of carbon in the mixed feed = (4*3.41+5*83.63+6*55.01+7*3.65) kmol/hr

= 787.4 kmol/hr

Now taking steam to carbon ratio as 3:1

Total steam needed = 3× 787.4 kmol/hr

= 2362.2 kmol/hr

Reactions in the reformer are

$C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$ ………. 1

$C_5H_{12} + 5H_2O \rightarrow 5CO + 11H_2$ ……….. 2

$C_6H_{14} + 6H_2O \rightarrow 6CO + 13H_2$ ……….. 3

$C_7H_{16} + 7H_2O \rightarrow 7CO + 15H_2$ ……….4

From the reaction 1

C_4H_{10} consumed = (0.65*3.41) = 2.217 kmol/hr

C_4H_{10} unconverted= (3.41– 2.217) = 1.193 kmol/hr

H_2O consumed = (4×2.217) = 8.868 kmol/hr

CO produced = (4×2.217) =8.868 kmol/hr

H_2 produced = (9×2.217) = 19.953 kmol/hr

From the reaction 2

C_5H_{12} consumed = (0.65× 83.63) kmol/hr =54.36 kmol/hr

C_5H_{12} unconverted= (83.63– 54.36) = 29.27 kmol/hr

H_2O consumed = 5× 54.36= 271.8 kmol/hr

CO produced =5× 54.36= 271.8 kmol/hr

H_2 produced = 11× 54.36= 597.96 kmol/hr

From the reaction 3

C_6H_{14} consumed = 0.65 × 55.01= 35.757 kmol/hr

C_6H_{14} unconverted = (55.01- 35.757) = 19.253 kmol/hr

H_2O consumed = (6 ×35.757) = 214.542 kmol/hr

CO produced = (6 ×35.757) = 214.542 kmol/hr

H_2 produced = (13×35.757) = 464.84 kmol/hr

From the reaction 4

C_7H_{16} consumed = 0.65 × 3.65= 2.373 kmol/hr

C_7H_{16} unconverted = (3.65-2.373) = 1.27 kmol/hr

H_2O consumed = (7 ×2.373) = 16.61kmol/hr

CO produced = (7 ×2.373) = 16.61kmol/hr

H_2 produced = (15×2.373) = 35.595 kmol/hr

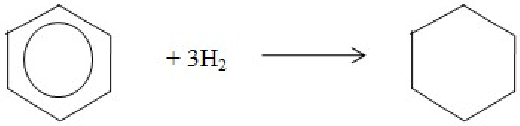
Total CO produced from all the three reactions = 511.82 kmol/hr

Total H_2O consumed from all the three reactions = 511.82 kmol/hr

Total H_2 produced from all the three reactions = 1118.348 kmol/hr

Total H_2O remaining = (2362.2 − 511.82) kmol/hr = 1850.38 kmol/hr

In addition, one more reaction will take place in the reformer, which is conversion of benzene to cyclohexane by adding hydrogen to benzene in presence of Ni catalyst which is also used for the reforming process. The hydrogen required for this process is got from the hydrogen produced in the reactions (1), (2), (3),(4). As the amount of benzene in feed is small, we assume that all the benzene is converted to cyclohexane.



Here,

Benzene consumed = 3.18 kmol/hr

Hydrogen used = 3×3.18 = 9.54 kmol/hr

Cyclobenzene produced = 3.18 kmol/hr

Therefore, hydrogen outlet from the reformer = (1118.348 −9.54) = 1108.8 kmol/hr

Input to the reformer considering recycle

Table 5.1

Component	**Moles(kmol/hr)**	**Molecular weight**	**Mass(kg/hr)**
C_4H_{10}	3.41	58	197.78
C_5H_{12}	83.63	72	6021.36
C_6H_{14}	55.01	86	4730.86
C_7H_{16}	3.65	100	365
N_2	5.5929	28	156.601
Benzene	3.18	78	248.04
Steam	2362.2	18	42519.6
Total			54239.2

Output from the reformer table 5.2

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0

Steam	1850.38	18	33306.84
CO	511.82	28	14330.96
CO2	0	44	0
H2	1108.8	2	2217.6
Cyclobenzene	3.18	84	267.12
Total			54239.2

∴ Input = Output.

5.4 MATERIAL BALANCE OVER THE SHIFT REACTOR

Reaction taking place

$CO + H_2O \rightarrow CO_2 + H_2$

Assuming 55% conversion of CO takes place

CO inlet = 511.82 kmol/hr

CO converted = 0.55× 511.82 = 281.501 kmol/hr

CO outlet = 230.319 kmol/hr

H_2O consumed = 281.501 kmol/hr

CO_2 produced = 281.501 kmol/hr

H_2 produced = 281.501 kmol/hr

H_2O outlet= (1850.38−281.501) = 1568.879 kmol/hr

CO_2 outlet = (281.501) kmol/hr

H_2 outlet = (281.501+1108) = 1390.309 kmol/hr

Input to the shift reactor (table 5.3)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0
Steam	1850.38	18	33306.84
CO	511.82	28	14330.96
CO2	0	44	0
H2	1108.8	2	2217.6
Cyclobenzene	3.18	84	267.12
Total			54239.2

Output from the shift reactor (table 5.4)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0
Steam	1568.879	18	28239.82
CO	230.319	28	6448.932
CO2	281.501	44	12386.04
H2	1390.309	2	2780.602
Cyclobenzene	3.18	84	267.12

Total			54239.2

5.5 MATERIAL BALANCE OVER WATER SEPARATOR

Water coming out as condensate = 1568.879 kgmol/hr = 28239.82 kg/hr

Also solubility of cyclobenzene is 213 mg/L at 25 °C. As the amount of cyclobenzene is very small, so we consider that all the cyclobenzene (267.12 kg/hr) gets dissolved in water and comes out with it.

Input to the water separator(table 5.5)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0
Steam	1568.879	18	28239.82
CO	230.319	28	6448.932
CO2	281.501	44	12386.04
H2	1390.301	2	2780.602
Cyclobenzene	3.18	84	267.12
Total			54239.2

Output from the water separator (table 5.6)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127

N_2	5.5929	28	156.6012
Benzene	0	78	0
CO	230.319	28	6448.932
CO2	281.501	44	12386.04
H2	1390.301	2	2780.602
Total			25731.57

25731.57+ 28239.82 + 267.12= Output = Input

5.6 MATERIAL BALANCE OVER CO_2 ABSORBER:

Assuming 95% of the CO_2 is absorbed in MEDA, we get

CO_2 inlet = 281.501 kmol/hr

CO_2 absorbed = 281.501× 0.95 = 267.426 kmol/hr = 11766.744 kg/hr

CO_2 outlet = 14.075 kmol/hr

Input to the CO_2 absorber: table 5.7

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0
CO	230.319	28	6448.932
CO2	281.501	44	12386.04
H2	1390.301	2	2780.602
Total			25731.57

Output from the CO_2 absorber: table 5.8

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Benzene	0	78	0
CO	230.319	28	6448.932
CO2	14.075	44	619.3
H2	1390.301	2	2780.602
Total			13964.83

11766.744 + 13964.83 = 25731.57 = Output = Input

5.7 MATERIAL BALANCE OVER PSA I:

Assumption

i) 100% CO, CO_2, C_4H_{10}, C_5H_{12}, C_6H_{14}, C_7H_{16}, N_2 absorbed.
ii) 0 % hydrogen absorbed.

So, hydrogen obtained is 2780 kg/hr.

Input to the PSAI: table 5.9

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
CO	230.319	28	6448.932
CO2	14.075	44	619.3
H2	1390.301	2	2780.602

Total			13964.83

Output from the PSAI: (table 5.10)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
CO	230.319	28	6448.932
CO2	14.075	44	619.3
Total			11184

2780 + 11184 = 13964.83 = Output = Input

5.8 MATERIAL BALANCE OVER PSA II:

Assumption

i) Assuming 100% absorption of C_4H_{10}, C_5H_{12}, C_6H_{14}, C_7H_{16}, N_2

ii) Assuming 0% absorption of CO, CO_2.

So, CO, CO_2 removed = (6448.932 + 619.3) = 7068.232 kg/hr

Input to the PSAII: (table 5.11)

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758

C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
CO	230.319	28	6448.932
CO2	14.075	44	619.3
Total			11184

Output from the PSA II: table 5.12

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	1.193	58	69.194
C_5H_{12}	29.27	72	2107.44
C_6H_{14}	19.253	86	1655.758
C_7H_{16}	1.27	100	127
N_2	5.5929	28	156.6012
Total			4115.993

7068.232 + 4115.993 = 11184 kg/hr = Output = Input

5.9 OVERALL MATERIAL BALANCE table 5.13

Component	Input		Output	
	Kmol/hr	Kg/hr	Kmol/hr	Kg/hr
C_4H_{10}	2.26	131.08	0.021	1.218
C_5H_{12}	55.4	3988.8	0.514	37.008
C_6H_{14}	36.56	3144.16	0.336	28.896
C_7H_{16}	2.5	250	0.021	2.1
N_2	0.1	2.8	0.1	2.8
Benzene	3.18	248.04	0	0
Steam	2362.2	42519.6	1568.879	28239.822
CO			230.319	6448.932
CO2			14.075 267.426	12386
H2			1390.301	2780.602
Cyclobenzene			3.18	267.12
Total		50284		50284

5.10 OVERALL CONVERSION OF THE PROCESS-

C_4H_{10}------13 moles of H_2

C_5H_{14}------16 moles of H_2

C_6H_{14}------19 moles of H_2

C_7H_{16}------22 moles of H_2

Theoretical H_2 produced at 100%=(13*2.26+16*55.4+19*36.56+22*2.5)

=1665.42

H_2 produced=1390.301

% conversion=(1390.301/1665.42)*100%

=83.48%

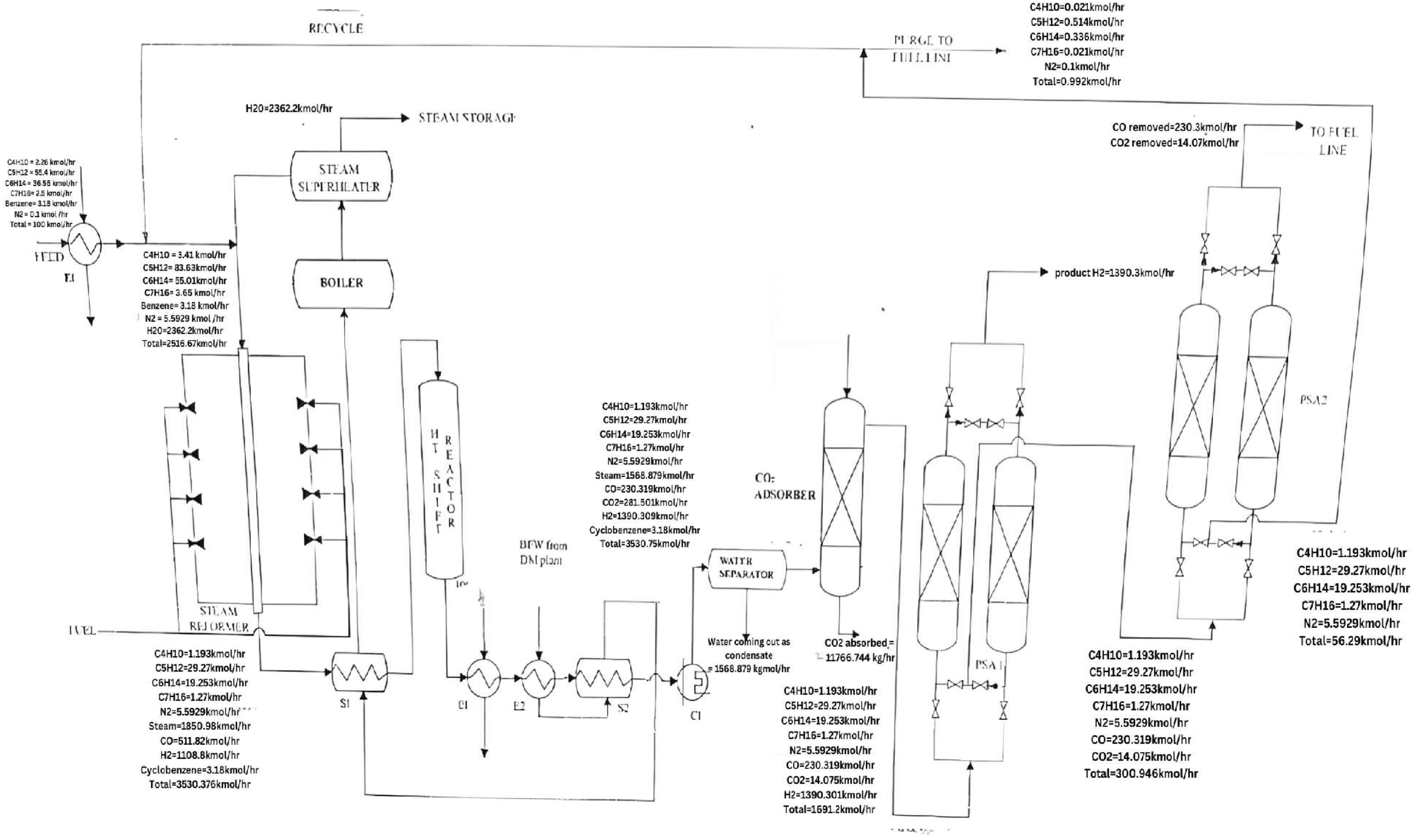


FIG 5.1—PROCESS FLOW DIAGRAM (MATERIAL BALANCE)

CHAPTER 6

MODIFIED MATERIAL BALANCE

- Basis 50000 tons of hydrogen gas produced.
- Assuming 335 working days per year

$$\frac{50000 * 1000}{335 * 24 * 2}$$

=3109.45kgmol/hr

Therefore multiplying factor=3109.45/1390.301

=2.23

6.1 MATERIAL BALANCE OVER REFORMER-

TABLE 6.1 Input to the reformer-

Component	**Kmol/hr**	**Molecular weight**	**Mass kg/hr**
C_4H_{10}	5.0398	58	292.3084
C_5H_{12}	123.542	72	8895.024
C_6H_{14}	81.5288	86	7011.4768
C_7H_{16}	5.575	100	557.5
N_2	0.223	28	6.244
Benzene	7.0914	78	553.1292
Steam	5267.706	18	94818.708

TABLE 6.2 Input to the reformer considering recycle-

Component	**Moles(kmol/hr)**	**Molecular weight**	**Mass(kg/hr)**
C_4H_{10}	7.6043	58	441.0494
C_5H_{12}	186.4949	72	13427.6328
C_6H_{14}	122.6723	86	10549.8178

C_7H_{16}	8.1395	100	813.95
N_2	12.4721	28	349.22
Benzene	7.0914	78	553.1292
Steam	5267.706	18	94818.708
Total			120953.5072

TABLE 6.3 Output from the reformer

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
Steam	4126.3474	18	74274.2532
CO	1141.3586	28	31958.0408
CO2	0	44	0
H2	2472.624	2	4945.248
Cyclobenzene	7.0914	84	595.6776

Total			120951.7942

6.2 MATERIAL BALANCE OVER SHIFT REACTOR-

TABLE 6.4 Input to the shift reactor

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
Steam	4126.3474	18	74274.2532
CO	1141.3586	28	31958.0408
CO2	0	44	0
H2	2472.624	2	4945.248
Cyclobenzene	7.0914	84	595.6776
Total			120951.7942

TABLE 6.5 Output from the shift reactor

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21

N_2	12.47	28	349.22
Benzene	0	78	0
Steam	3498.60017	18	62974.80306
CO	513.611	28	14381.11
CO2	627.74723	44	27620.87812
H2	3100.38	2	6200.77814
Cyclobenzene	7.0914	84	595.6776
Total			120951.8215

6.3 MATERIAL BALANCE OVER WATER SEPARATOR

TABLE 6.6 Input to the water separator

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
Steam	3498.60017	18	62974.80306
CO	513.611	28	14381.11
CO2	627.74723	44	27620.87812
H2	3100.38	2	6200.77814
Cyclobenzene	7.0914	84	595.6776
Total			120951.8215

TABLE 6.7 Output from the water separator

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
CO	513.611	28	14381.11
CO2	627.74723	44	27620.87812
H2	3100.38	2	6200.77814
Total			57381.37084

STEAM at outlet =3498.60017kmol/hr=62974.80306kg/hr

Cyclobenzene at outlet=7.0914kmol/hr=595.6776 kg/hr

6.4 MATERIAL BALANCE OVER CO_2 ABSORBER:

TABLE 6.8 Input to the CO2 absorber:

Component	Moles (kmol/hr)	Molecular weight	Mass (kg/hr)
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
CO	513.611	28	14381.11
CO2	627.74723	44	27620.87812
H2	3100.38	2	6200.77814

Total			57381.37084

TABLE 6.9 output from the CO2 absorber:

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Benzene	0	78	0
CO	513.611	28	14381.11
CO2	31.387	44	1381.039
H2	3100.38	2	6200.77814
Total			31141.5709

CO_2 at outlet=26239.83912

<u>6.5 MATERIAL BALANCE OVER PSA I</u>:

TABLE 6.10 Input to the PSAI

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22

CO	513.611	28	14381.11
CO2	31.387	44	1381.039
H2	3100.38	2	6200.77814
Total			31141.5709

TABLE 6.11 Output from PSAI

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
CO	513.611	28	14381.11
CO2	31.387	44	1381.039
Total			24940.32

6.6 MATERIAL BALANCE OVER PSA II:

TABLE 6.12 Input to the PSAII

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22

CO	513.611	28	14381.11
CO2	31.387	44	1381.039
Total			24940.32

TABLE 6.13 Output from PSAII

Component	**Moles (kmol/hr)**	**Molecular weight**	**Mass (kg/hr)**
C_4H_{10}	2.66	58	154.3026
C_5H_{12}	65.27	72	4699.502
C_6H_{14}	42.93	86	3692.34
C_7H_{16}	2.83	100	283.21
N_2	12.47	28	349.22
Total			9178.66439

6.7 PURGE STREAM-

Purge stream=1 kmol/hr

Mole fraction of C4H10 in the purge stream =0.021*2.23*1=0.04683

Mole fraction of C5H12 in the purge stream=0.514*2.23*1=1.14622

Mole fraction of C6H14 in the purge stream=0.336*2.23*1=0.74928

Mole fraction of C7H16 in the purge stream=0.021*2.23*1=0.04683

Mole fraction of N2 in the purge stream=0.1*2.23*1=0.223

CHAPTER 7

ENERGY BALANCE

7.1 ENERGY BALANCE OVER REFORMER--

Heat exchanger 1

Let, temperature of the feed at heat exchanger outlet br ‘T’.

Heat gained by the feed stream = $\int_{298}^{T}(mCp\ dT)$

$\Delta H = \int mc_p dT$

$$= \int_{298}^{T}(mCpdT)_{C4H10} + \{\int_{298}^{309.25}(mCpdT)_{C5H12} + [mC_5H_{12} \times \text{ latent heat}] + \int_{309.25}^{T}(mCpdT)_{C5H12}\} + \{\int_{298}^{342.05}(mCpdT)_{C6H14} + [mC_6H_{14} \times \text{ latent heat}] + \int_{342.05}^{T}(mCpdT)_{C6H14}\} + \{\int_{298}^{371.57}(mCpdT)_{C7H16} + [mC_7H_{16} \times \text{ latent heat}] + \int_{371.57}^{T}(mCpdT)_{C7H16}\} + \{\int_{298}^{353.25}(mCpdT)_{C6H6} + [mC_6H_6 \times \text{ latent heat}] + \int_{353.25}^{T}(mCpdT)_{C6H6}\} + \int_{298}^{T}(mCpdT)_{N2}$$

Heat lost by water = $\int_{473}^{433}(mCp\ dT)$ H20

= (-5625165) kJ/hr

Here, m_{H20} = 4755.7 kmol/hr

Heat lost by the steam = 5625165 kJ/hr = Heat gained by the feed= ΔH

By try and error method we get T= 373 K

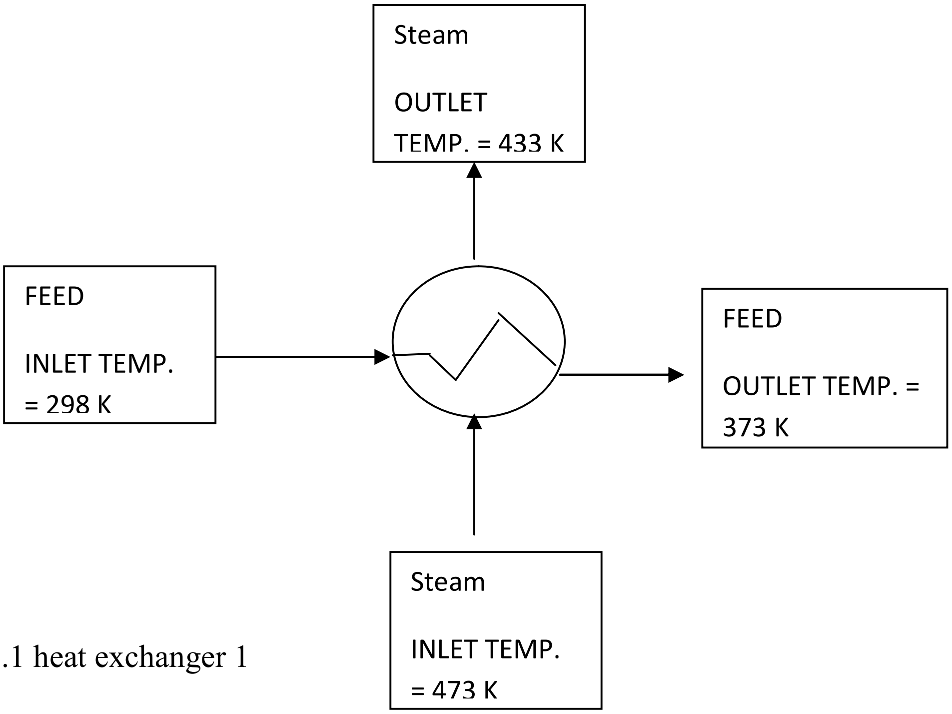


FIG 7.1 heat exchanger 1

7.1.1 ENERGY BALANCE OVER MIX POINT 1

Total enthalpy of the feed stream –

$$\Delta H = \int mc_p dT$$

$$= \int_{298}^{373} (mCpdT)_{C4H10} + \{\int_{298}^{309.25} (mCpdT)_{C5H12} + [mC_5H_{12} \times \text{ latent heat}]$$
$$+ \int_{309.25}^{373} (mCpdT)_{C5H12}\} + \{\int_{298}^{342.05} (mCpdT)_{C6H14} + [mC_6H_{14} \times \text{ latent heat}]$$
$$+ \int_{342.05}^{373} (mCpdT)_{C6H14}\} + \{\int_{298}^{371.57} (mCpdT)_{C7H16} + [mC_7H_{16} \times \text{ latent heat}]$$
$$+ \int_{371.57}^{373} (mCpdT)_{C7H16}\} + \{\int_{298}^{353.25} (mCpdT)_{C6H6} + [mC_6H_6 \times \text{ latent heat}]$$
$$+ \int_{353.25}^{373} (mCpdT)_{C6H6}\} + \int_{298}^{373} (mCpdT)_{N2}$$

$\Delta H = 5625364.57$ KJ/hr

Where,

mC_4H_{10}= 5.0398 kmol/hr

mC_5H_{12}=123.542 kmol/hr

mC_6H_{14}=81.5288 kmol/hr

mC_7H_{16}=5.575 kmol/hr

mC_6H_6=7.0914 kmol/hr

mN_2= 0.223 kmol/hr

Latent Heat

Pentane= 26.4 KJ/Kg

Hexane = 365 KJ/Kg

Heptane= 318 KJ/KG

Benzene= 393.2 KJ/Kg

Total enthalpy of the recycle stream

$\Delta H = \int mc_p dT$

$$=\int_{298}^{353}(mCpdT)_{C4H10}+\int_{298}^{353}(mCpdT)_{C5H12}+\int_{298}^{353}(mCpdT)_{C6H14}+\int_{298}^{353}(mCpdT)_{C7H16}+\int_{298}^{353}(mCpdT)_{N2}$$

= 804834.56307 KJ/Kg

Where,

mC_4H_{10}= 2.565 kmol/hr

mC_5H_{12}=62.953 kmol/hr

mC_6H_{14}=41.144 kmol/hr

mC_7H_{16}= 2.565 kmol/hr

mN_2= 12.249 kmol/hr

Let "T" be the temperature of the stream after mixing, then by heat balance

Enthalpy oh the feed stream + Enthalpy oh the recycle stream = 6430199.133 KJ/hr

$$\therefore 6430199.133 \text{ KJ/hr} = \int_{298}^{T}(mCpdT)_{C4H10} + \int_{298}^{T}(mCpdT)_{C5H12} + \int_{298}^{T}(mCpdT)_{C6H14} + \int_{298}^{T}(mCpdT)_{C7H16} + \int_{298}^{T}(mCpdT)_{N2} + \int_{298}^{T}(mCpdT)_{C6H6}$$

Where,

mC_4H_{10} = 7.604 kmol/hr

mC_5H_{12} = 186.495 kmol/hr

mC_6H_{14} = 122.672 kmol/hr

mC_7H_{16}=8.14 kmol/hr

Benzene= 7.091 kmol/hr

mN_2 = 12.472 kmol /hr

By try and error method, the equation is solved and we get the mix feed temperature, T= 425.2855 K.

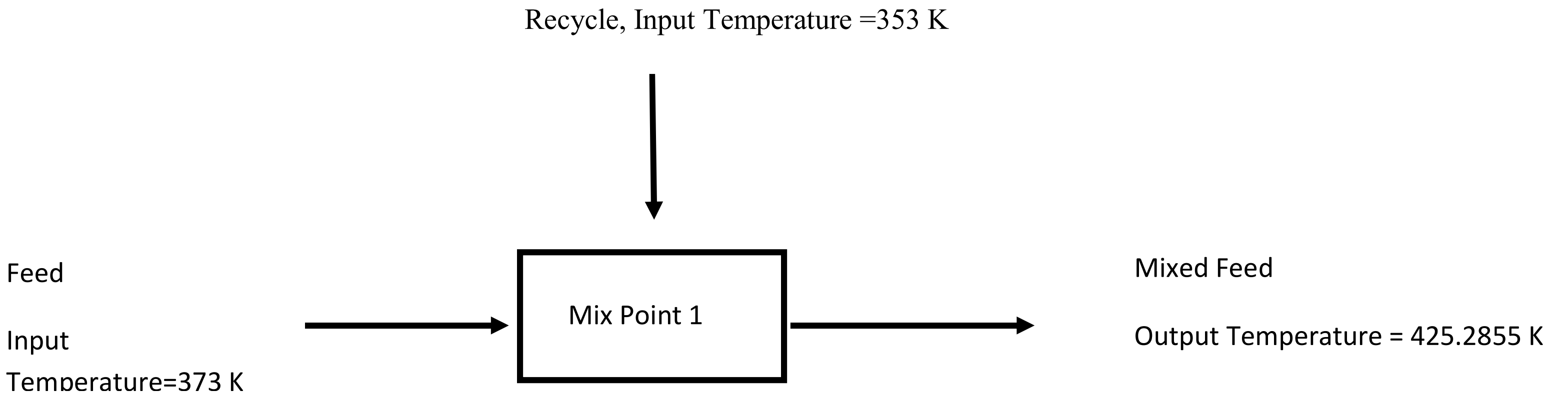


FIG 7.2- mix point 1

7.1.2 ENERGY BALANCE OVER MIX POINT 2

Total enthalpy of the mixed feed stream –

$\Delta H = \int_{298}^{T}(mCpdT)_{C4H10} + \int_{298}^{T}(mCpdT)_{C5H12} + \int_{298}^{T}(mCpdT)_{C6H14} + \int_{298}^{T}(mCpdT)_{C7H16} + \int_{298}^{T}(mCpdT)_{N2} + \int_{298}^{T}(mCpdT)_{C6H6}$

ΔH= 6430199.133 KJ/hr

Where,

mC_4H_{10} = 7.604 kmol/hr

mC_5H_{12} = 186.495 kmol/hr

mC_6H_{14} = 122.672 kmol/hr

mC_7H_{16}=8.14 kmol/hr

Benzene= 7.091 kmol/hr

mN_2 = 12.472 kmol /hr

Let, the temperature of the superheated steam is 200°C

Flow rate of the superheated steam = 5267.706 kmol/hr

Enthalpy of stream $= \int_{298}^{473}(mCpdT)_{H2O}$

= 27054800.04053 KJ/Kg

$(Cp)_{H2O} = 30.869 - 1.9\times 10^{-2}T + 2.79\times10^{-5}T^2 - 1.27\times10^{-8} T^3$

Let 'T' be the temperature after mixing mixed feed and steam, therefore

Enthalpy of the mixed feed stream + Enthalpy of the steam = (6430199.133 +27054800.04053) = 33484999.17 KJ/Kg

$$\therefore 33484999.17 = \int_{298}^{T}(mCpdT)_{C4H10} + \int_{298}^{T}(mCpdT)_{C5H12} + \int_{298}^{T}(mCpdT)_{C6H14} + \int_{298}^{T}(mCpdT)_{C7H16} + \int_{298}^{T}(mCpdT)_{N2} + \int_{298}^{T}(mCpdT)_{C6H6} + \int_{298}^{T}(mCpdT)_{H2O}$$

By try and error method, the equation is solved and we get the stream temperature after mix point 2, T= 459.8514K.

Where,

mC_4H_{10} = 7.604 kmol/hr

mC_5H_{12} = 186.495 kmol/hr

mC_6H_{14} = 122.672 kmol/hr

mC_7H_{16}=8.14 kmol/hr

Benzene= 7.091 kmol/hr

mN_2 = 12.472 kmol /hr

mH_2O = 5267.706 kmol /hr

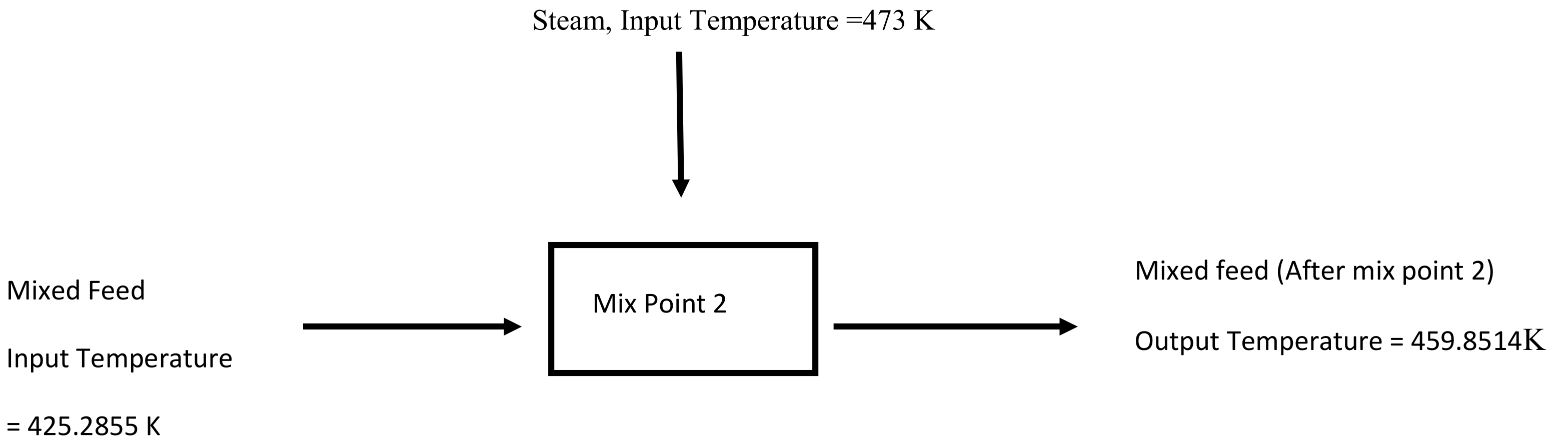


FIG 7.3-mix point 2

7.1.3 ENERGY BALANCE OVER REFORMER

Enthalpy of the stream after mix point 2, entering reformer =33484999.17 KJ/Kg

Temperature of the stream after mix point 2, entering reformer = 459.8514 K

The reactions in the reformer occurs at the temperature of 800°C

Reactions occurring in the reformer are –

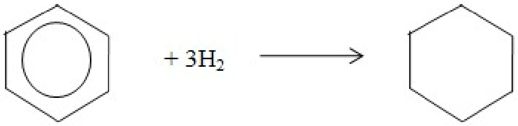
$C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$ ………. 1

$C_5H_{12} + 5H_2O \rightarrow 5CO + 11H_2$ ……….. 2

$C_6H_{14} + 6H_2O \rightarrow 6CO + 13H_2$ ……….. 3

$C_7H_{16} + 7H_2O \rightarrow 7CO + 15H_2$ ……….4

And



……5

Standard heat of reaction at 298 K

Reaction 1

$\Delta H^\circ_{298} = \sum(H^\circ)_{PRODUCT} - \sum(H^\circ)_{REACTANT}$

$= [4(-110525)+9(0)]-[4\times(-241818)+(-125790)]$

$= 650962$ kJ

Reaction 2

$\Delta H^\circ_{298} = \sum(H^\circ)_{PRODUCT} - \sum(H^\circ)_{REACTANT}$

$=[5(-125790)+11(0)]-[5\times(-241818)+(-146760)]$

$=803225$ kJ

Reaction 3

$\Delta \mathbf{H}^\circ_{298} = \sum (\boldsymbol{H}^\circ)_{\text{PRODUCT}} - \sum (\boldsymbol{H}^\circ)_{\text{REACTANT}}$

=[6(-125790)+13(0)]−6×(-241818)+(-166940)

=954698 kJ

Reaction 4

$\Delta \mathbf{H}^\circ_{298} = \sum (\boldsymbol{H}^\circ)_{\text{PRODUCT}} - \sum (\boldsymbol{H}^\circ)_{\text{REACTANT}}$

=[7(-125790)+15(0)]−7×(-241818)+(-187781)

= 624415 kJ

Reaction 5

$\Delta \mathbf{H}^\circ_{298} = \sum (\boldsymbol{H}^\circ)_{\text{PRODUCT}} - \sum (\boldsymbol{H}^\circ)_{\text{REACTANT}}$

=[-123145]−[3×(0)+82930]

= -206075 kJ

Heat of reaction

Reaction 1

$\Delta \mathbf{H}_{\mathbf{R1}} = (\int_{459.851}^{298} (mCpdT)_{\text{reactant}}) + \Delta \mathbf{H}^\circ_{298} + (\int_{298}^{1073} (mCpdT)_{\text{product}}$

=7918697.46607 kJ/hr

For 65% conversion $\Delta \mathbf{H}_{\mathbf{R1}}$= 5147153.05 kj/kg

Reaction 2

$\Delta \mathbf{H}_{\mathbf{R2}} = (\int_{459.851}^{298} (mCpdT)_{\text{reactant}}) + \Delta \mathbf{H}^\circ_{298} + (\int_{298}^{1073} (mCpdT)_{\text{product}}$

=239123564.2636 kJ/hr

For 65% conversion $\Delta \mathbf{H}_{\mathbf{R2}}$= 155430316.6 kj/kg

Reaction 3

$\Delta\mathbf{H}_{\mathbf{R3}}$ = $(\int_{459.851}^{298}(mCpdT)$ reactant$)+ \Delta\mathbf{H}°_{\mathbf{298}} + (\int_{298}^{1073}(mCpdT)$ product

= 186729561.18613 kJ/hr

For 65% conversion $\Delta\mathbf{H}_{\mathbf{R1}}$= 121374214.8 kj/kg

Reaction 4

$\Delta\mathbf{H}_{\mathbf{R4}}$ = $(\int_{459.851}^{298}(mCpdT)$ reactant$)+ \Delta\mathbf{H}°_{\mathbf{298}} + (\int_{298}^{1073}(mCpdT)$ product

= 10422329.46306 kJ/hr

For 65% conversion $\Delta\mathbf{H}_{\mathbf{R4}}$= 6774514.149 kj/kg

Reaction 5

$\Delta\mathbf{H}_{\mathbf{R5}}$ = $(\int_{459.851}^{298}(mCpdT)$ reactant$)+ \Delta\mathbf{H}°_{\mathbf{298}} + (\int_{298}^{1073}(mCpdT)$ product

= -807094.26287 kJ/hr

For 65% conversion $\Delta\mathbf{H}_{\mathbf{R5}}$= -524611.27 kj/kg

Therefore,

$\Delta\mathbf{H}_{\mathbf{R\ 1073}}$ = 288201587.3 Kj/kg

Heat Output $=\int_{298}^{1073}(mCpdT)_{C4H10} + \int_{298}^{1073}(mCpdT)_{C5H12} + \int_{298}^{1073}(mCpdT)_{C6H14} + \int_{298}^{1073}(mCpdT)_{C7H16} + \int_{298}^{1073}(mCpdT)_{N2} + \int_{298}^{1073}(mCpdT)_{C6H6} + \int_{298}^{1073}(mCpdT)_{H2O} + \int_{298}^{1073}(mCpdT)_{CO} + \int_{298}^{1073}(mCpdT)_{C6H12}$

= 240194001.4 Kj/kg

Where,

Component	Kmol/hr
C_4H_{10}	1.193
C_5H_{12}	29.27
C_6H_{14}	19.253
C_7H_{16}	1.27
N_2	5.5929
Benzene	0
Steam	1850.38
CO	511.82
CO2	0
H2	1108.8
Cyclobenzene	3.18

<u>Heat balance over the reformer</u>

Heat input by the mixed stream +Heat input given in the form of fuel = Heat output + Heat used in the reaction.

$\therefore$ 33484999.17+ h = 240194001.4 + 288201587.3

$\therefore$ Heat given in the form of feed (h) = 494910589.5 KJ/hr

Input		Output	
Mixed stream	33484999.17	Out stream	240194001.4
Fuel	494910589.5	Output Reaction	288201587.3
Total	494910589	Total	494910589

Table 7.1

7.2 STEAM BALANCE OVER STEAM DRUM-

Let m be the rate of cooling water used in Kmol/hr

Now, heat lost by hot stream will be equal to the heat gained by cold stream

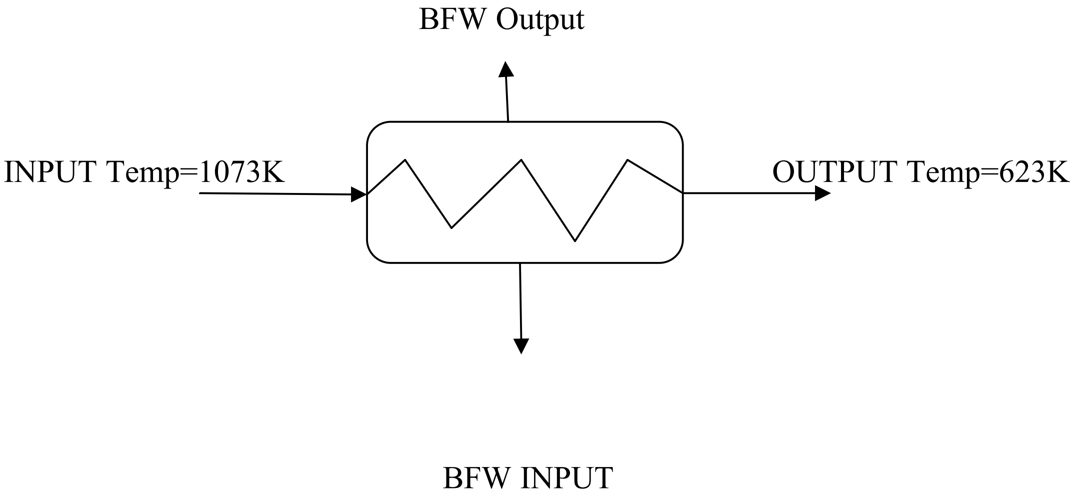


FIG-7.4 energy balance over the steam drum

Heat lost by hot stream=$(\int_{623}^{1073} mCpdt)_{C_4H_{10}}+\int_{623}^{1073} mCpdt)_{C_5H_{14}}+\int_{623}^{1073} mCpdt)_{C_6H_{14}}+\int_{623}^{1073} mCpdt)_{C_7H_{16}}+\int_{623}^{1073} mCpdt)_{CO}+\int_{623}^{1073} mCpdt)_{H_2}+\int_{623}^{1073} mCpdt)_{H_2O}+\int_{623}^{1073} mCpdt)_{C_6H_{12}}+\int_{623}^{1073} mCpdt)_{N_2}$

=147692864.9 Kmol/hr

Heat gained by the cold stream $=m*\lambda_{H2O}$

m*40657=147692864.9

m=3632.65 kmol/hr

λ=latent heat of vapourization

7.3 ENERGY BALANCE OVER HT-SHIFT REACTOR:

The reaction taking place is-

$$CO + H_2O \longrightarrow CO_2 + H_2$$

Assuming the extent of reaction to be only 55%.

The standard heat of reaction is-

$\Delta H^\circ_{298} = (\sum H^\circ)_{PRODUCT} - (\sum H^\circ)_{REACTANT}$

= -393509-(-110525-241818)

= -41166 KJ / Kmol

Heat of reaction,

$$\Delta H_R = (\int_{623}^{298} mCpdT)_{REACTANT} + m\Delta H^\circ_{298} + (\int_{298}^{700} mCpdT)_{PRODUCT}$$

$$= (\int_{623}^{298} mCpdT)_{H_2O} + (\int_{623}^{298} mCpdT)_{CO} + m\Delta H^\circ_{298} + (\int_{298}^{700} mCpdT)_{CO_2}$$

$$+ (\int_{298}^{700} mCpdT)_{H_2}$$

= -21503550.68 KJ / hr

Heat input to HT-Shift reactor $= (\int_{298}^{623} mCpdT)_{H_2O} + (\int_{298}^{623} mCpdT)_{C_4H_{10}}$

$+ \quad (\int_{298}^{623} mCpdT)$ C_5H_{12} $+ \quad (\int_{298}^{623} mCpdT)$ C_6H_{14} $+ \quad (\int_{298}^{623} mCpdT)$ C_7H_{16} $+$ $(\int_{298}^{623} mCpdT)$ H_2 $+ (\int_{298}^{623} mCpdT)$ CO $+ (\int_{298}^{623} mCpdT)$ N_2 $+ (\int_{298}^{623} mCpdT)$ C_6H_{12}

= 92553603.43 KJ / hr

Heat output from reactor = $(\int_{298}^{700} mCpdT)$ H_2O $+ (\int_{298}^{700} mCpdT)$ C_4H_{10}

$+ \quad (\int_{298}^{700} mCpdT)$ C_5H_{12} $+ \quad (\int_{298}^{700} mCpdT)$ C_6H_{14} $+ \quad (\int_{298}^{700} mCpdT)$ C_7H_{16} $+$ $(\int_{298}^{700} mCpdT)$ H_2 $+ (\int_{298}^{700} mCpdT)$ CO_2 $+ (\int_{298}^{700} mCpdT)$ CO $+ (\int_{298}^{700} mCpdT)$ N_2 $+ (\int_{298}^{700} mCpdT)$ C_6H_{12}

= 120189293.1 KJ / hr

Heat Balance over reactor,

Heat input + Heat used up in reaction = Heat output + Heat removed

Therefore, Heat removed = -6132139 KJ/hr

INPUT(KJ/hr)		OUTPUT(KJ/hr)	
Input stream	92553603.43	Output stream	120189293.1
Input reaction	21503550.68	Heat removed	-6132139
Total	114057154.1	Total	114057154.1

Table 7.2

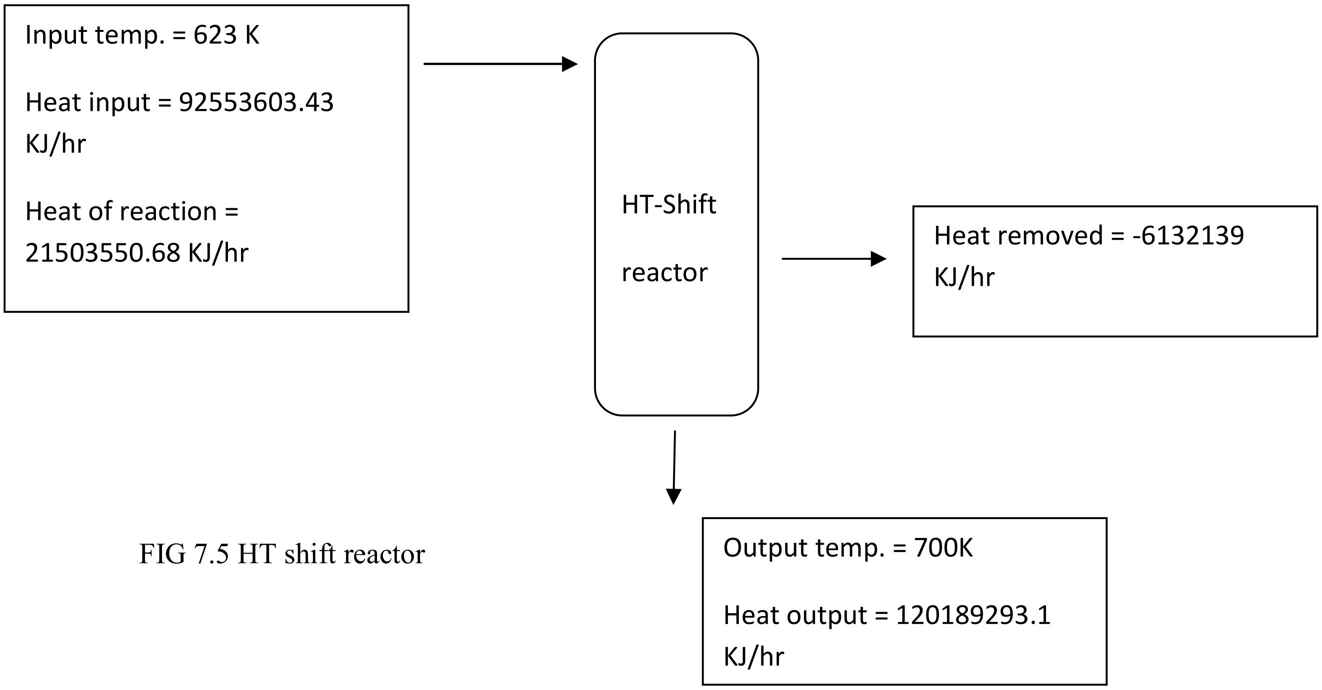


FIG 7.5 HT shift reactor

7.4 ENERGY BALANCE OVER HEAT EXCHANGER E2:

Let the temperature of feed at exchanger be T.

Heat lost by feed stream = $(\int_T^{700} mCpdT)$

$$= (\int_T^{700} mCpdT)_{H_2O} + (\int_T^{700} mCpdT)_{C_4H_{10}}$$

$$+ (\int_T^{700} mCpdT)_{C_5H_{12}} + (\int_T^{700} mCpdT)_{C_6H_{14}} + (\int_T^{700} mCpdT)_{C_7H_{16}} + (\int_T^{700} mCpdT)_{H_2} + (\int_T^{700} mCpdT)_{CO_2} + (\int_T^{700} mCpdT)_{CO} + (\int_T^{700} mCpdT)_{N_2} + (\int_T^{700} mCpdT)_{C_6H_{12}}$$

Let, mass of water be 5000 kmol/hr.

Heat gained by water stream = $(\int_{298}^{373} mCpdT)$ water

$= 28230894.968$ KJ/hr

Therefore, by trial and error method,

$T = 633.29$ K

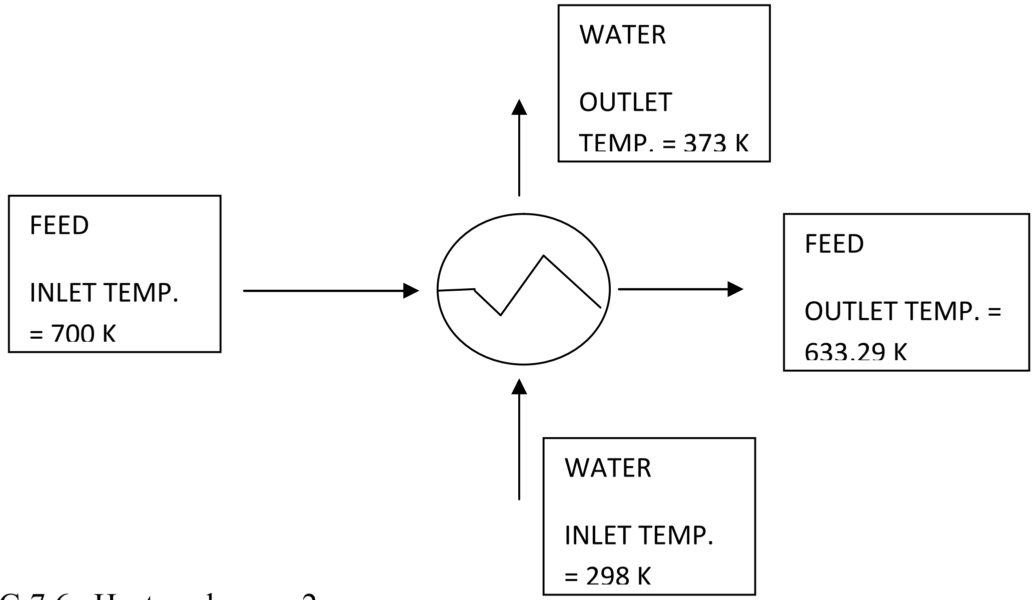


FIG 7.6 –Heat exchanger 2

7.5 ENERGY BALANCE OVER HEAT EXCHANGER E3:

Let the temperature of feed at exchanger be T.

Heat lost by feed stream = $(\int_{T}^{633.9} mCpdT)$

$$= (\int_{T}^{633.9} mCpdT)_{H_2O} + (\int_{T}^{633.9} mCpdT)_{C_4H_{10}}$$

$$+ (\int_{T}^{633.9} mCpdT)_{C_5H_{12}} + (\int_{T}^{633.9} mCpdT)_{C_6H_{14}} + (\int_{T}^{633.9} mCpdT)_{C_7H_{16}} + (\int_{T}^{633.9} mCpdT)_{H_2} + (\int_{T}^{633.9} mCpdT)_{CO_2} + (\int_{T}^{633.9} mCpdT)_{CO} + (\int_{T}^{633.9} mCpdT)_{N_2} + (\int_{T}^{633.9} mCpdT)_{C_6H_{12}}$$

Let, mass of water be 5000 kmol/hr.

Heat gained by water stream = $(\int_{298}^{373} mCpdT)$ water

= 28230894.968 KJ/hr

Therefore, by trial and error method,

T = 559.13 K

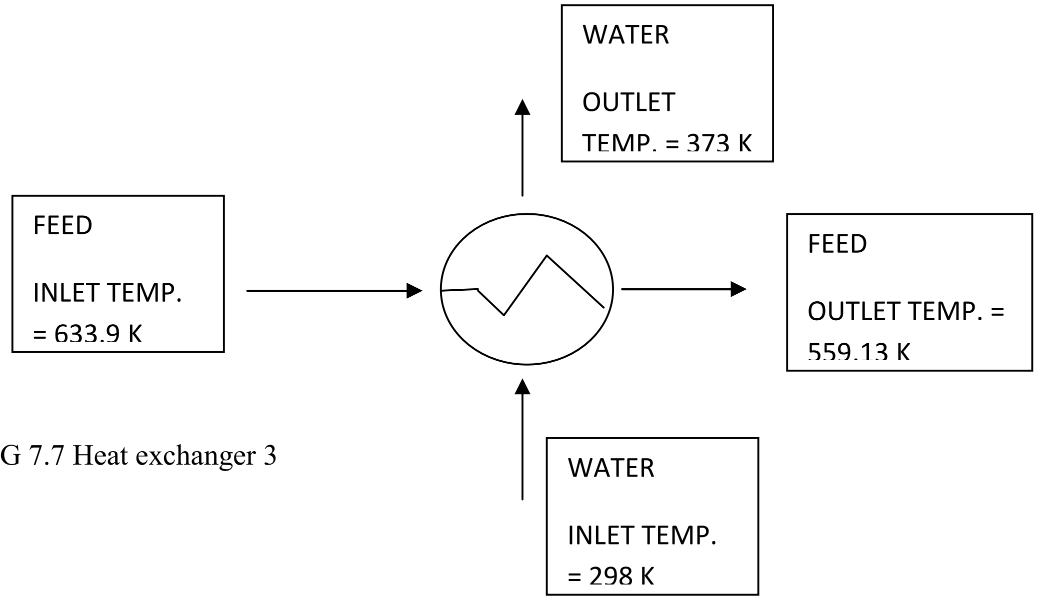


FIG 7.7 Heat exchanger 3

7.6 ENERGY BALANCE OVER STEAM DRUM 2:

Heat lost by HT-Shift reactor in steam drum = Heat gained by steam drum 2

Heat lost by HT-Shift reactor in steam drum = $\int_{390}^{559.13} mCpdT$

= $(\int_{390}^{559.13} mCpdT)$ H_2O + $(\int_{390}^{559.13} mCpdT)$ C_4H_{10}

$+ \ (\int_{390}^{559.13} mCpdT)\ C_5H_{12} \ + \ (\int_{390}^{559.13} mCpdT)\ C_6H_{14} \ + \ (\int_{390}^{559.13} mCpdT)\ C_7H_{16} \ +$
$(\int_{390}^{559.13} mCpdT)\ H_2 \ + \ (\int_{390}^{559.13} mCpdT)\ CO_2 \ + \ (\int_{390}^{559.13} mCpdT)\ CO \ + \ (\int_{390}^{559.13} mCpdT)\ N_2 \ +$
$(\int_{390}^{559.13} mCpdT)\ C_6H_{12}$

=

Assuming latent heat of vaporization of water, λ_{H_2O} = 40657 J/mol

Now, by heat balance,

$$\int_{390}^{559.13} mCpdT = m \times \lambda_{H_2O}$$

So, m = 1231.94 Kmol/hr

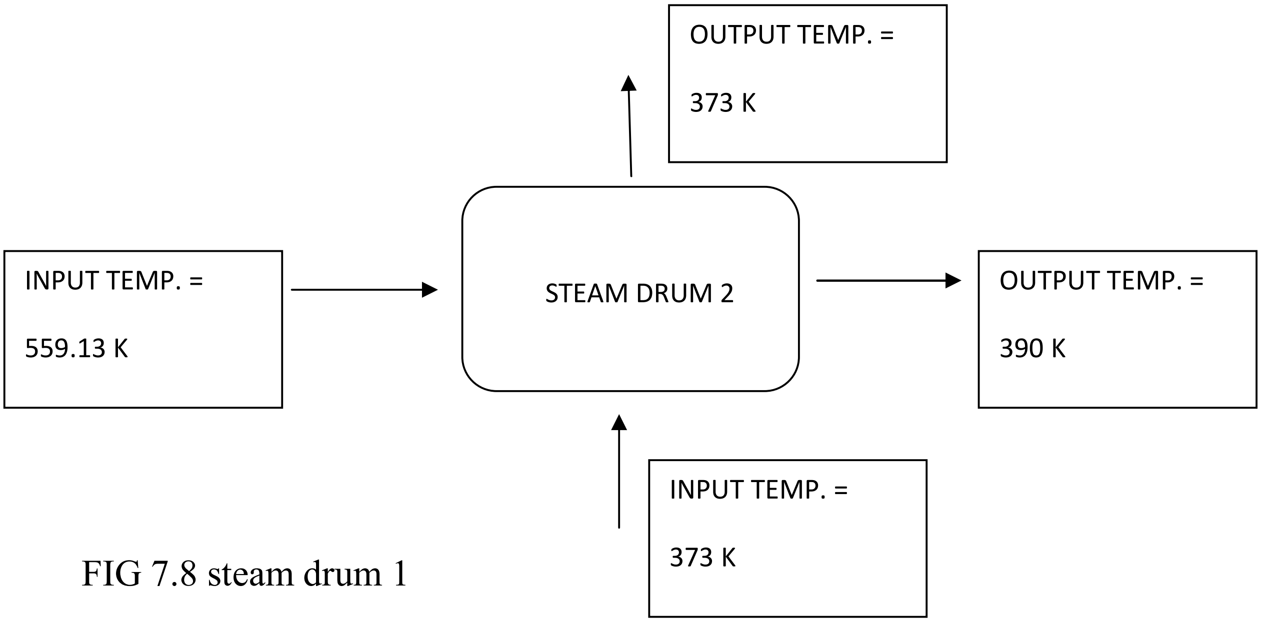


FIG 7.8 steam drum 1

<u>7.7 ENERGY BALANCE OVER COOLER:</u>

Here, we need to calculate the flow rate of cooling water used to exchange the heat.

Let it be m.

Let, the hot stream be cooled from 390K TO 353K.

Heat lost by hot stream = $(\int_{353}^{390} mCpdT)_{H_2O} + (\int_{353}^{390} mCpdT)_{C_4H_{10}}$

$+ (\int_{353}^{390} mCpdT)_{C_5H_{12}} + (\int_{353}^{390} mCpdT)_{C_6H_{14}} + (\int_{353}^{390} mCpdT)_{C_7H_{16}} + (\int_{353}^{390} mCpdT)_{H_2} + (\int_{353}^{390} mCpdT)_{CO_2} + (\int_{353}^{390} mCpdT)_{CO} + (\int_{353}^{390} mCpdT)_{N_2} + (\int_{353}^{390} mCpdT)_{C_6H_{12}}$

= 10338332.62 KJ/hr

Heat gained by cold stream = $(\int_{298}^{333} mCpdT)_{water}$ = m × 2623.55

Thus, Heat lost = Heat gained

⇒ 10338332.62 = m × 2623.55

By solving, m = 3940.589 Kmol/hr

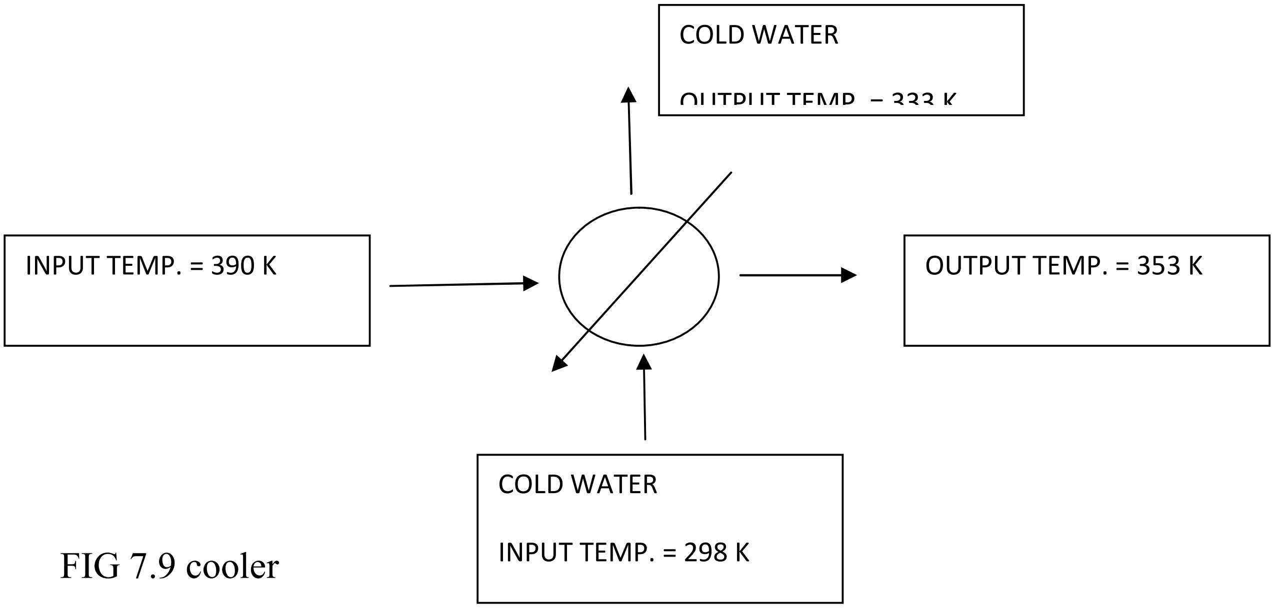


FIG 7.9 cooler

7.8 ENERGY BALANCE OVER WATER SEPARATOR-

Heat input to the water separator=

$=(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{CO}+$ $\int_{298}^{353} mCpdt)_{CO2}+\int_{298}^{353} mCpdt)_{H2}+\int_{298}^{353} mCpdt)_{H2O}+\int_{298}^{353} mCpdt)_{C6H12}+\int_{298}^{353} mCpdt)_{N2}$

=15411.402+464286.59124+363971.37043+28036.94148+818093.72476+1006886.20276+6537221.60531+5617209.86499+45321.59850+23228.82457

=14919668.13 KJ/hr

Heat output of stream entering CO2 absorber

$=(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{CO}+$ $\int_{298}^{353} mCpdt)_{CO2}+\int_{298}^{353} mCpdt)_{H2}+\int_{298}^{353} mCpdt)_{N2}$

=9257136.667 KJ/hr

Heat output of condensate stream=5662531.463

Total heat output=5662531.463+9302458.265

=14919668.13KJ/hr

So total heat input=total heat output

Table 7.3 Energy balance over the water separator

Input stream(Kj/hr)	14919668.13	Out stream(Kj/hr)	9257136.667
		condensate(Kj/hr)	5662531.463
total(Kj/hr)	14919668.13	total(Kj/hr)	14919668.13

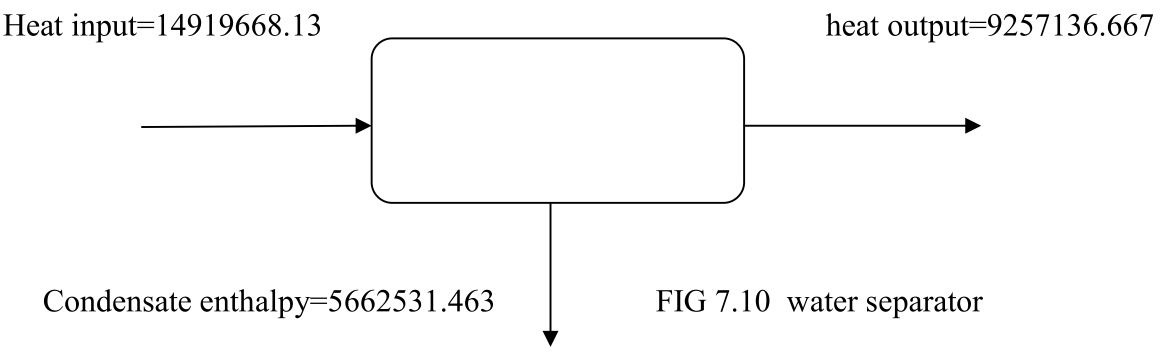


FIG 7.10 water separator

7.9 ENERGY BALANCE OVER CO2 ABSORBER

Heat input to the system from water separator=

$$=(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{CO}+\int_{298}^{353} mCpdt)_{CO2}+\int_{298}^{353} mCpdt)_{H2}+\int_{298}^{353} mCpdt)_{N2}$$

=9257136.667 KJ/hr

Heat output of stream entering PSAI

$$=(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{CO}+\int_{298}^{353} mCpdt)_{CO2}+\int_{298}^{353} mCpdt)_{H2}+\int_{298}^{353} mCpdt)_{N2}$$

=8300594.195 KJ/hr

Heat output of absorbed carbon stream=956542.4725 KJ/hr

Total heat output=956542.4725+8300.594.195

=9257136.667 KJ/hr

So,Total heat input=total heat output

Table 7.4 Energy balance over the CO2 absorber

INPUT(KJ/hr)		OUTPUT(KJ/hr)	
Input stream	9257136.667	Out stream	8300594.195
		Absorbed stream	956542.4725
total	9257136.667	total	9257136.667

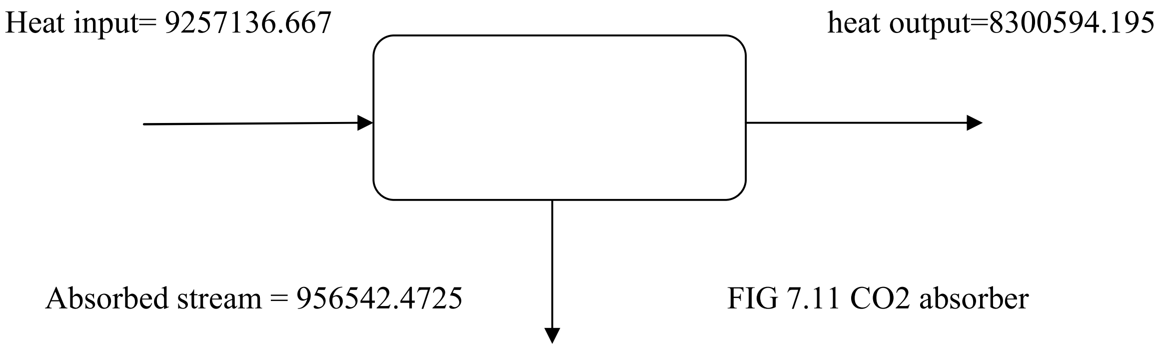


FIG 7.11 CO2 absorber

7.10 ENERGY BALANCE OVER PSA-I

Enthalpy input to PSAI=8300594.195 KJ/hr

Enthalpy of H_2 stream from PSAI=$\int_{298}^{353} mCpdt)_{H2}$

=6537221.605 KJ/hr

Enthalpy of stream entering PSAII from PSAI

$$==(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{CO}+\int_{298}^{353} mCpdt)_{CO2}+\int_{298}^{353} mCpdt)_{N2}$$

=1763372.59 KJ/hr

Total enthalpy output=6537221.605+1763372.59

=8300594.195 KJ/hr

Therefore, total heat input=total heat output

Table 7.5 Energy balance over the PSAI

INPUT(KJ/hr)		OUTPUT(KJ/hr)	
Input stream	8300.594.195	Out stream	1763372.59
		Absorbed stream	6537221.605
total	8300.594.195	total	8300594.195

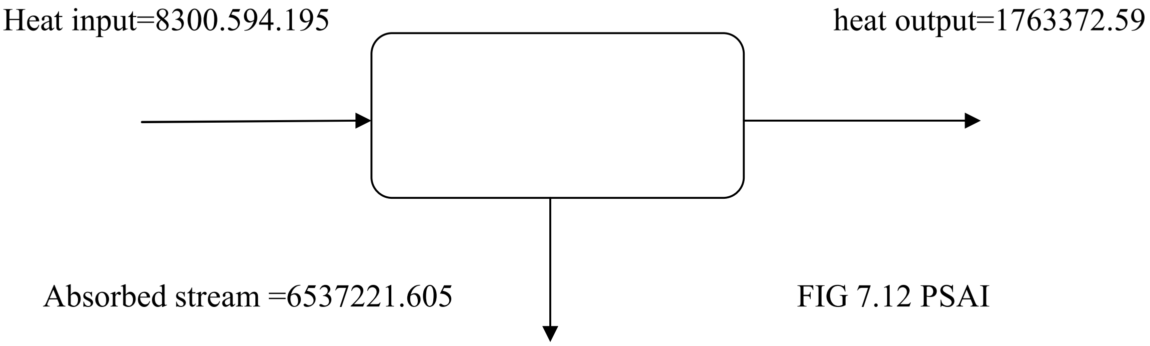


FIG 7.12 PSAI

7.11 ENERGY BALANCE OVER PSA-II

Enthalpy input to PSAII=1763372.59 KJ/hr

Enthalpy of C_4H_{10}, C_5H_{12}, C_6H_{14}, C_7H_{16}, N_2 stream

$=(\int_{298}^{353} mCpdt)_{C4H10}+\int_{298}^{353} mCpdt)_{C5H14}+\int_{298}^{353} mCpdt)_{C6H14}+\int_{298}^{353} mCpdt)_{C7H16}+\int_{298}^{353} mCpdt)_{N2}$

=894935.8641 KJ/hr

Enthalpy of CO, CO_2 stream

$=\int_{298}^{353} mCpdt)_{CO}+\int_{298}^{353} mCpdt)_{CO2}$

=868437.450 KJ/hr

Total enthalpy output=1763372.59 KJ/hr

Therefore, total enthalpy input=total enthalpy output

Table 7.6 Energy balance over the PSAII

INPUT(KJ/hr)		OUTPUT(KJ/hr)	
Input stream	1763372.59	Out stream	894935.8641
		Absorbed stream	868437.450
total	1763372.59	total	1763372.59

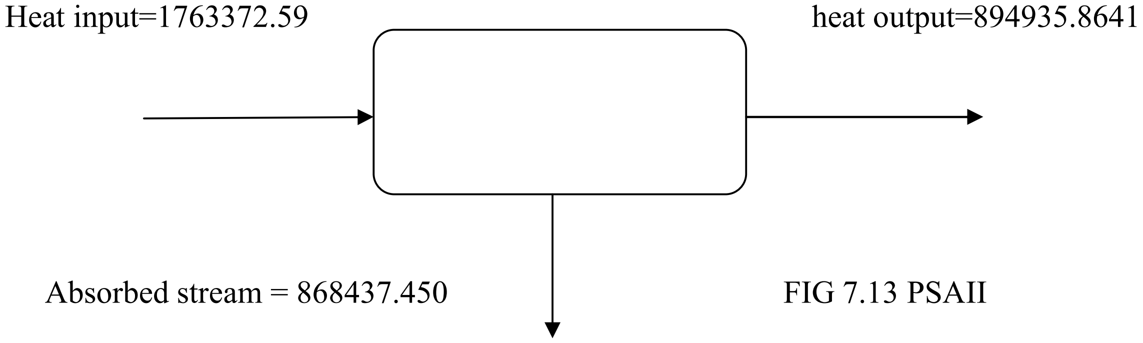


FIG 7.13 PSAII

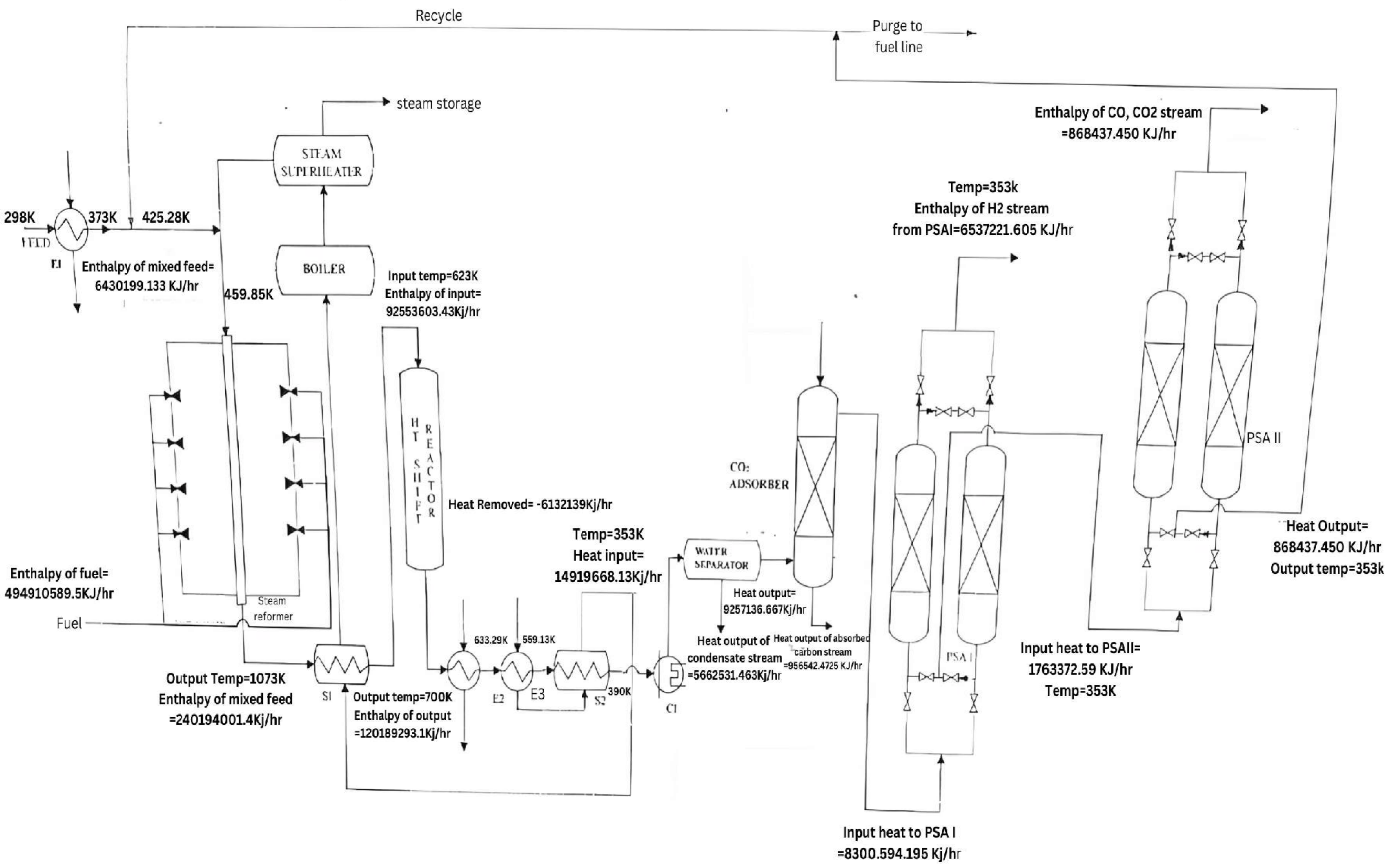


FIG 7.13 PROCESS FLOW DIAGRAM (ENERGY BALANCE)

CHAPTER 8

EQUIPMENT DESIGN

8.1 HEAT EXCHANGER-

STEP1-

ASSUMPTION

Shell side	Tube side
ID=23 1/4	Number and length=364,8'0''
Baffle space =12 in	OD, BWG, pitch=3/4in,16 BWG 15/16 in, tri
Passes=1	Passes=2

STEP 2-

Q_{hot}=26757725.5724 Btu/hr

Q_{cold}=26757725.5724 Btu/hr

STEP 3-

	HOT FLUID	COLD FLUID	DIFFERENCE
HIGHER TEMPERATURE	800.33	211.73	588.73
LOWER TEMPERATURE	680.2	76.73	603.47
DIFFERENCES	120.6	135	14.4

ALL DATA's ARE TAKEN FROM D Q KERN

ΔT_1=603.47

ΔT_2=588.73

R=0.889

S=0.186

LMTD=596.01°F F_t=0.98

Δt=584.0898°F

UD=100 (table 8)

A=Q/(UD*LMTD)=400 ft^2

Since 400 >200 ft^2

Therefore, 1-2 shell and tube heat exchanger is used

STEP-4—

μ_{hot}=0.02<1 Cp

μ_{cold}=0.95<1 Cp

Therefore, T_{avg} are used for each stream

T_{avg}=740.2°F

T_{avg}=144.23°F

STEP-5—Property table

PROPERTY	**HOT SIDE**	**COLD SIDE**
Cp(fig 2)	0.904	1.1
μ(Fig 15)(lb/ft-hr)	0.0532	1.1616
K(table 5)(BTU/ft °F-hr)	0.0364	0.381
S(table 6)	1.795	1
P(lb/ft^3)	112.187	62.5

Step6: h_o and h_i calculation:

Hot Fluid	Cold fluid
a_s= ID×CB'/144×P	$a_{t'}$ = 0.302 ft^2

$= \frac{21.25\times0.188\times12}{144\times0.75}$ $= 0.355\ \text{ft}^2$ Steam is passed through the tube side and the mixed feed is passed through the shell side. G_s= W/ as = 266653.06/0.355 lb/hr-ft2 =7511.3.38 lb/hr-ft^2 $D_e = \frac{0.55}{12}$ = 0.0458 ft (From fig28) $Re = \frac{D\times Gs}{\mu}$ =646654.143 J_H = 520(From figure 28) $h_o= \frac{JH\ k}{De}\ (\frac{Cp\ \mu}{k})^{\frac{1}{3}}$ = 453.48 Btu/hr$-ft^2$°F	$a_t = \frac{Nt \times at'}{144\times n}$ = 0.382 G_t = (198416.04/0.382) lb/hr-ft^2 = 519413.717 lb/hr-ft2 $V_t = \frac{Gt}{3600\times\rho}$ = 2.657 ft/hr $D = \frac{0.62}{12}$ =0.052 ft $Re = \frac{D\times Gt}{\mu}$ = 23251..99 J_H = 70(From figure 28, Appendix, DQ Kern) $h_i= \frac{JH\ k}{D}\ (\frac{Cp\ \mu}{k})^{\frac{1}{3}}$ = 767.705 Btu/hr$-ft^2$°F $h_{io} = h_{i*}\frac{ID}{OD}$ =243.336Btu/hr$-ft^2$°F

Step 7:U_c calculation

$$U_c = \frac{hio \times hi}{hio + hi}$$

= 264.48

∴ $U_D < U_c$

Dirt factor= $(\frac{1}{UD} - \frac{1}{Uc})$ = 0.006

Pressure drop Calculation

Shell Side	Tube side
Assuming $\phi_{s=}$ 1 Re=646654.143 $D_s = \frac{21,25}{12} = 1.77$ f = 0.0009 ft^2/in^2 Specific heat, S = 1.795 No of crosses = N+ 1 = $\frac{12L}{B}$ $= \frac{12\times8}{12}$ = 8 $\Delta P_s = \frac{f\ Gs^2 Ds\ (N+1)}{5.22\times10^{10} De\quad \phi s}$ $= \frac{0.009\times(751135.38)^2\times1.77\times8}{5.22\times10^{10}\times0.0458\times1.795}$ = 1.675 psi < 10 psi	Assuming $\phi_{t=}$ 1 Re=23251..99 f = 0.00023 ft^2/in^2 S = 1 $V_t =$ 2.657 ft/hr $\Delta P_t = \frac{f\ Gt^2 Ln}{5.22\times10^{10} DS\ \phi t}$ = 0.366 psi G_t = 519413.717 lb/hr-ft^2 $\therefore \frac{Vt^2}{2\ g'}$ =0.035 $\Delta P_r = \frac{4n}{s}\frac{Vt^2}{2\ g'}$ = 0.28 psi $\Delta P_T = \Delta P_r + \Delta P_t$ = 0.646 < 10 psi

8.2 DESIGN OF PRESSSURE VESSEL AND HEAD

Assumption:

MOC IS 2002:1962 grade 2B quality steel

ID=1500mm

J=0.85 (Double welded butt joint)

Disc shaped head is used
Pressure=405 Kpa
Therefore, Design pressure, Pw=1.05*405=425.565KPa
Thickness= t =P di/(2fj-P)=3.18mm
Corrosion allowance=1.5mm
Therefore actual thickness=3.18+1.5=4.68mm
Standard thickness=5mm

Let, Ri=Do, r_o=0.6Do, S_f=40mm

f=118*10^6 N/m^2

Assume, Ri = Ro = Do

Now we have calculate effective height,

h_E = 0.206m (minimum value)

h_E /Do=0.137

$\frac{t}{D0}$ = pc/2fj = (405*10^3C)/(2*118*0.85)

=1.7* 10^{-3} C

From table 4.1(B), IS 2825-1969, code book

C=3

Therefore= t/Do =6mm

Now, 6mm+1.5+6% (thinning allowance)= 7.95

= 8mm (standard)

Assumption verification: Di=Do-2t=1484

t/Di=0.0539<0.25

Therefore, our assumption is correct

Assumptions:

1. MOC IS 2002:1962 grade 28 quality steel
2. 1D = 1.5m = 1500mm
3. Double welded butt joint with full penetration Le I = 0.85
4. No severe condition is assumed.
5. Disc shaped head is used

Pressure-405.3 KPa

Therefore, design pressure,

p = 1.03*Pw = 1.05 * 405.3 = 425.565KPa

Thickness, $t = \frac{Pdi}{2fj - P}$ …….1

($f = 118 \times 10^6\ n/m^2$ Appendix A, table A-1, page 261)

$$t = \frac{425.565 \times 10^2 \times 1500}{(2 \times 118 \times 10^6 \times 0.85) - (425.565 \times 10^2)} = 3.18 \text{ mm}$$

Corrosion allowances= 1.5 mm

Therefore actual thickness = 3.18 – 1.5 = 4.68 mm

Standard thickness = 5mm (Appendix B, page 269)

Let,

$R_i = D_o,\ r_o = 0.6D,\ S_f = 40\text{mm}$

Now we have,

P=405.3 kPa, f= f= $118 \times 10^6\ N/m^2$, D_o= 1.5m

Thickness, $t = \frac{PDoC}{2fj}$ ………1

Since C is a function of ‘t”, first assumption,

$R_i = R_o = Do$

Now we have to calculate the effective external height of the head and for this, We have, $h_E = \mathrm{Ro} - [(\mathrm{Ro} - \frac{\mathrm{Do}}{2}) \times (\mathrm{Ro} + \frac{\mathrm{Do}}{2}) - 2\mathrm{ro}]^{0.5}$

$$= 1.5 - [(1.5 - \frac{1.5}{2}) \times (1.5 + \frac{1.5}{2}) - 2 \times 0.6]^{0.5}$$

$$= 0.206 \text{ m}$$

Or, $\frac{\mathrm{Do}^2}{4\times \mathrm{Ro}} = 0.375$ m

$(\frac{\mathrm{Do\ ro}}{2})^2 = 0.259$ m

Among the three values, the minimum value is 0.206m Hence the effective external height of the head is 0.206.

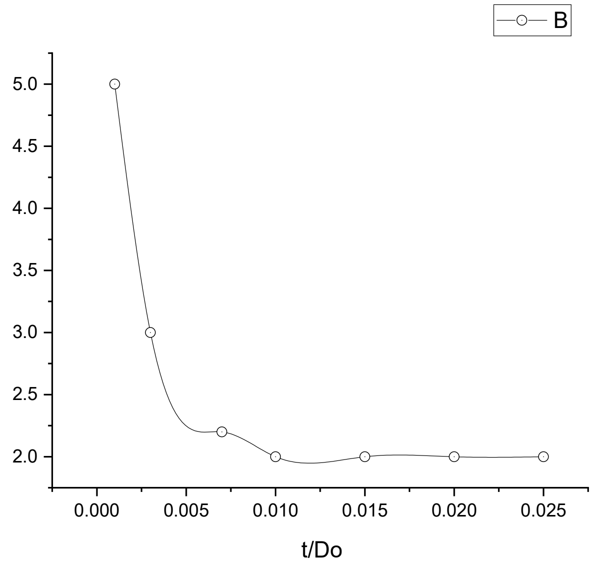
Again, $h_E / \mathrm{Do} = 0.137$

As the diameter of the veesel (1.5m) is not very large, the head can be fabricated from a single plate. Therefore, J=1

From equation 1

$$\frac{t}{\mathrm{Do}} = \frac{\mathrm{PC}}{2fj} = \frac{405.3\times10^3}{2\times118\times10^6} = 1.7 \times 10^{-3}\mathrm{C}$$

From the figure 3.7 IS 2825-1969, page20, code book and by plotting the curve between C versus $\frac{t}{\mathrm{Do}}$ a value of c=3 is obtained.



Therefore, $\frac{t}{\mathrm{Do}} = 6\times 10^{-3}\ mm$

If corrosion allowance of 1.5 mm is added to that, the required uncorroded plate thickness will be 8.5 mm If 6% allowance is given then a standard plate thickness of 10 mm will be compared to 1.5, 10 mm is very small. Hence the first assumption $R1 = R_0$ does not introduce any considerable error in result.

CHAPTER-9

CONCLUSION

The demand for hydrogen is growing in many industries, particularly in the chemical and refining industries. The process of steam reforming has been active in this field for more than 50 years and offers a wide range of advanced technologies for small and large capacities meeting the demand for low operating and investment costs. Advanced steam reformer design allows high temperatures and low steam to carbon ratios for hydrogen production resulting in high energy efficiency and lower cost plants.

Looking at the environmental benefits of using hydrogen as fuel, it is found that it burning of hydrogen with air under proper conditions result in low harmful emissions. Besides, reduction in NO, emissions is possible with a lower combustion temperature. Using hydrogen as a fuel allows the advent of many renewable energy sources in the near future in the fuel sector.

In place of naphtha steam reforming, its time to switch over to or adopt natural gas reforming as a better alternative. Though naphtha steam reforming is an economic one, the later is not.

REFERENCES

1. Process heat transfer by Donald . Q .Kern

2. Equipment design by B.C.Bhattacharya

3. Mass transfer operation by Dr. B.K.Dutta

4. Chemical Reaction Engineering by Octave Levenspiel

5. Stoichiometry and Process Calculations by K.V.Narayanan and B.Lakshmikutty

6. Acar C, Dincer I “Comparative assessment of hydrogen production methods from renewable and non-renewable sources” International Journal of Hydrogen Energy 39 (2014)

7. Steam Naphtha Reforming by the Imperial Chemical Industries Process Raymond J. Kenard, Jr. Joseph C. Maggins

8. Pavlos Nikolaidis , Andreas Poullikkas, 2017, “Renewable and Sustainable Energy Reviews”, Energy policy 67, 597-611

9. www.wikipedia.com/SteamReformingofNaphtha

APPENDIX I

Heat of Formation of Materials

Standard Heat of Formation of different components at 298K are given. All components are at gaseous state at this temperature.

C_4H_{10}, $(\Delta H^{\circ}_{298}) = -125790$ KJ / Kg mol

C_5H_{12}, $(\Delta H^{\circ}_{298}) = -146760$ KJ / Kg mol

C_6H_{14}, $(\Delta H^{\circ}_{298}) = -166940$ KJ / Kg mol

C_7H_{16}, $(\Delta H^{\circ}_{298}) = -187780$ KJ / Kg mol

CO_2, $(\Delta H^{\circ}_{298}) = -393509$ KJ / Kg mol

CO, $(\Delta H^{\circ}_{298}) = -110525$ KJ / Kg mol

H_2O, $(\Delta H^{\circ}_{298}) = -241818$ KJ / Kg mol

H_2, $(\Delta H^{\circ}_{298}) = 0$ KJ / Kg mol

N_2, $(\Delta H^{\circ}_{298}) = 0$ KJ / Kg mol

C_6H_6, $(\Delta H^{\circ}_{298}) = 82930$ KJ / Kg mol

C_6H_{12}, $(\Delta H^{\circ}_{298}) = -123140$ KJ / Kg mol

APPENDIX II

C_P Values of different compounds-

Let, the ambient temperature be 298 K.

The equation for C_P is given by,

$$C_P = A + BT + CT^2 + DT^3 \text{ KJ / Kmol K},$$

where, T = Temperature, K

A, B, C, D are constants.

C_4H_{10} (GAS), $C_P = 9.487 + 3.31E\text{-}01T + -1.11E\text{-}04T^2 + -2.82E\text{-}09T^3$

C_5H_{12}(GAS) , $C_P = -3.626 + 4.87E\text{-}01T + -2.58E\text{-}04T^2 + 5.30E\text{-}08T^3$

C_6H_{14}(GAS) , $C_P = -4.41 + 5.82E\text{-}01T + -3.12E\text{-}04T^2 + 6.49E\text{-}08T^3$

CO_2(GAS) , $C_P = 31.15 + -1.36E\text{-}02T + 2.68E\text{-}05T^2 + -1.17E\text{-}08T^3$

CO(GAS) , $C_P = 27.143 + 9.27E\text{-}03T + -1.38E\text{-}05T^2 + 7.65E\text{-}09T^3$

H_2O(GAS) , $C_P = 30.869 + -1.29E\text{-}02T + 2.79E\text{-}05T^2 + -1.27E\text{-}08T^3$

H_2O(LIQUID) , $C_P = 18.2964 + 4.72E\text{-}01T + -1.34E\text{-}03T^2 + 1.31E\text{-}06T^3$

H_2(GAS) , $C_P = 19.795 + 7.34E\text{-}02T + 5.6E\text{-}05T^2 + 1.72E\text{-}08T^3$

N_2(GAS) , $C_P = 32.243 + 1.92E\text{-}03T + 1.06E\text{-}05T^2 + -3.6E\text{-}09T^3$

C_7H_{16}(GAS) , $C_P = 26.984 + 5.03E\text{-}01T + -4.47E\text{-}05T^2 + -1.68E\text{-}07T^3$

C_6H_6(GAS) , $C_P = -31.368 + 4.74E\text{-}01T + -3.11E\text{-}04T^2 + 8.52E\text{-}08T^3$

C_6H_{12}(GAS) , $C_P = 13.783 + 2.07E\text{-}01T + 5.36E\text{-}04T^2 + -6.3E\text{-}07T^3$

C_7H_{16}(LIQUID) , $C_P = 101.12 + 9.77E\text{-}01T + -3.07E\text{-}03T^2 + 4.18E\text{-}06T^3$

C_6H_6(LIQUID) , $C_P = -31.662 + 1.3E{+}00T + -3.6E\text{-}03T^2 + 3.82E\text{-}06T^3$