

DESIGN OF METHANOL PRODUCTION PROCESS

A Report

submitted by

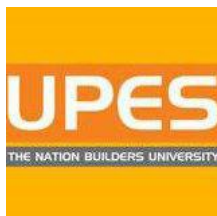
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*in partial fulfillment of the requirements
for the award of the degree of*

BACHELOR OF TECHNOLOGY
in
CHEMICAL ENGINEERING
with specialization in
REFINING & PETROCHEMICALS

Under the guidance of

Mr. Rahul Kumar
Assistant Professor



DEPARTMENT OF CHEMICAL ENGINEERING

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CERTIFICATE

This is to certify that the thesis titled **DESIGN OF METHANOL PRODUCTION PROCESS** submitted by CHINMAY VERMA, RHYTHM AGARWAL, NAYAN KALE, SHIVAM ASHOK DIXIT, to the University of Petroleum & Energy Studies, for the award of the degree of **BACHELOR OF TECHNOLOGY** in Chemical Engineering with specialization in Refining and Petrochemicals is a bonafide record of project work carried out by them under our supervision.

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NOMENCLATURE

L	Top Liquid Flow rate
V	Top Vapour Flow rate
\bar{L}	Bottom Liquid Flow rate
\bar{V}	Bottom Vapour Flow rate
ρ_v	Vapour Density
ρ_l	Liquid Density
M_{Avg}	Average Molecular Weight
$[P]$	Parachor Value
Ψ	Volumetric Flow rate
T_c	Critical Temperature
P_c	Critical Pressure
T	Temperature
V	Pressure
R	Universal Gas Constant
η	Efficiency
χ	Mole fraction
C_p	Specific Heat at Constant Pressure
C_v	Specific Heat at Constant Volume
T_r	Reduced Temperature
P_r	Reduced Pressure
A, B, C	Antoine Constants
α	Relative Volatility
x_D	Moles of more volatile in Distillate
x_w	Moles of more volatile in Bottoms
R_m	Minimum Reflux ratio
λ	Latent Heat of vapourization
N_m	Minimum Number of Trays

ABSTRACT

Global economic, environmental, and political forces have increased interest in developing sources of liquid transportation fuels that are not petroleum based. Renewable biomass has the potential to provide an alternative energy source that offers many advantages over petroleum. Biomass can be converted into synthesis gas by gasification, and the synthesis gas can be efficiently converted into methanol using existing technology. The traditional technology deals with very high pressures of about 600-1700 Psig and very high temperatures ranging between 400 – 500°C for the conversion. But, the process and catalyst selected in this paper operate at a temperature of about 260°C and 110 bar pressure.


In this paper, a process for conversion of synthesis gas to methanol has been identified and a process flow diagram is developed. Also, mass and energy balances have been applied to the selected process flow diagram along with the designing of the distillation tower to separate methanol and water using 400 TPD capacity as the basis of calculations. Further, a cost estimation for the distillation column has been done.

Key words: Syn gas, Methanol synthesis, Methanol-water separation, Methanol cost, Methanol demand.

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Chapter 1

Introduction

Global economic, environmental, and political forces have increased interest in developing sources of liquid transportation fuels that are not petroleum based. Renewable biomass has the potential to provide an alternative energy source that offers many long-term advantages over petroleum. Biomass can be converted into synthesis gas by gasification, and the synthesis gas can be efficiently converted into methanol using existing technology. It is possible that, in the not-to-distant future, most liquid-consuming transportation vehicles (cars, trucks, trains, and planes) may use methanol as their energy source. Olah et al. propose a methanol economy as a more practical approach compared to the widely discussed hydrogen economy because existing liquid fuel infrastructure (pipelines and tanks) could be used with little modification, and the safety concerns associated with hydrogen can be avoided.

This paper studies the process to convert synthesis gas into methanol. A cooled tubular reactor is used to react hydrogen with the carbon monoxide and carbon dioxide in the synthesis gas to produce methanol. Water is a byproduct. The gas-phase exothermic reactions are conducted in a packed tubular reactor, which is cooled by generating steam. A large gas recycle stream is required to obtain high overall conversion. A distillation column separates methanol from water.

A fixed amount of synthesis gas is fed into the system, and the effects of the many design optimization variables on the yield of methanol, the energy costs, and the capital costs are evaluated. These variables include reactor pressure, reactor size, concentration of inert components in the recycle gas, and pressure in a flash tank upstream of the column. The purpose of the flash tank is to keep light components from entering the

column that would blanket the condenser.

The investigation reveals that the economics are dominated by methanol yield. Energy costs and capital costs are an order of magnitude smaller than the value of the product. The major energy cost is compression of the synthesis gas, so the optimum reactor operating pressure is a trade-off between compression costs and methanol yield. Reactor temperature is set such that high-pressure steam can be produced in the reactor. Reactor size is a trade-off between reactor and catalyst capital investment, and recycle compression costs (energy and capital). Inert component concentration in the recycle gas is a trade-off between methanol yield (reactant losses in the vent) and compression costs. Selection of pressure in the flash tank is a trade-off between compressor costs in two compressors that are affected in opposite directions by varying the flash-tank pressure.



Chapter 2

Objectives

1. Designing a methanol production plant with a capacity of 400 TPD using synthesis gas as the raw material.
2. The designing includes consideration of all the technical and economic aspects of distillation column.



Chapter 3

Literature Review

In the embalming process, the ancient Egyptians used a mixture of substances, including methanol, which they obtained from the pyrolysis of wood. Pure methanol, however, was first isolated in 1661 by Robert Boyle, when he produced it via the distillation of buxus (boxwood). It later became known as "pyroxylic spirit". In 1834, the French chemists Jean-Baptiste Dumas and Eugene Peligot determined its elemental composition.

They also introduced the word "methylene" to organic chemistry, forming it from Greek methy = "wine" + hl = wood (patch of trees), with Greek language errors: "wood (substance)" (Greek xylon) was intended, and the components are in the wrong order for Greek. The term "methyl" was derived in about 1840 by back-formation from "methylene", and was then applied to describe "methyl alcohol". This was shortened to "methanol" in 1892 by the International Conference on Chemical Nomenclature. The suffix -yl used inorganic chemistry to form names of carbon groups, was extracted from the word "methyl".

In 1923, the German chemists Alwin Mittasch and Mathias Pier, working for BASF, developed a means to convert synthesis gas (a mixture of carbon monoxide, carbon dioxide, and hydrogen) into methanol. A patent was filed 12 January 1926 (reference no. 1,569,775). This process used a chromium and manganese oxide catalyst, and required extremely vigorous conditions pressures ranging from 50 to 220 atm, and temperatures up to 450°C. Modern methanol production has been made more efficient through use of catalysts (commonly copper) capable of operating at lower pressures. The modern low pressure methanol (LPM) was developed by ICI in the late 1960s with the technology now owned by Johnson Matthey, which is a leading licensor of methanol technology.

Methanol is one of the most heavily traded chemical commodities in the world, with an estimated global demand of around 27 to 29 million metric tons. In recent years, production capacity has expanded considerably, with new plants coming on-stream in South America, China and the Middle East, the latter based on access to abundant supplies of methane gas. Even though name plate production capacity (coal-based) in China has grown significantly, operating rates are estimated to be as low as 50 to 60%. No new production capacity is scheduled to come on-stream until 2015.

The use of methanol as a motor fuel received attention during the oil crises of the 1970s due to its availability, low cost, and environmental benefits. By the mid-1990s, over 20,000 methanol "flexible fuel vehicles" capable of operating on methanol or gasoline were introduced in the U.S. In addition, low levels of methanol were blended in gasoline fuels sold in Europe during much of the 1980s and early-1990s. Automakers stopped building methanol FFVs by the late-1990s, switching their attention to ethanol-fueled vehicles. While the methanol FFV program was a technical success, rising methanol pricing in the mid- to late-1990s during a period of slumping gasoline pump prices diminished the interest in methanol fuels.

Methanol Production feed stocks Methanol can and has been produced from a variety of substances over the years including: Wood Coal Natural gas Crop residues Grass Forest residues Cellulosic parts of municipal solid wastes.

Although all of these methods have been used at one time or another, today the main feedstock used for methanol production is natural gas. This is because it is the most cost effective, convenient, and effective method. Recently other biomass sources have been receiving attention as possible methanol production feedstock.

Chapter 4

Indian Scenario

There are five main producers of methanol in India:

Name Of the Manufacturer	Technology Licensor
Gujarat Narmada Valley Fertilizers Company Ltd (GNVFC)	ICI
Deepak Fertilizers	ICI
Assam Petrochemicals	ICI
Rashtriya Chemicals Fertilizers Limited	Haldor Topsoe
National Fertilizers Limited	Haldor Topsoe

TABLE 4.1: Methanol Producers in India

There are five units spread all over the country with licensed and installed capacities of 351,500 TPA and 301,500 TPA respectively. The production in 1988-89 was 145,000 MT. Haldia plant is not in operation.

There was appreciable import of methanol; 78,000 tonne in 1987-88 and 43,000 tonne in 1988-89; apparently there is no import in 1989-90 and 1990-91. The current demand of methanol is more than 200,000 tonne. This demand is expected to grow to around 300,000 tonne in 1994-95 and 425,000 tonne by 2000 AD, as per perspective plan projections.

The feedstock for the manufacturing units is Fuel oil/LSHS and Naphtha. Associated gas is now available to RCF at Trombay, and natural gas to both GNFC at Gujarat and Assam Petrochemicals Ltd., Assam.

Chapter 5

Process Comparison

Methanol is produced mainly from natural gas. Naphtha, fuel oil and coal are other suitable feedstocks. Modern industrial scale methanol production is based exclusively on synthesis gas mixture of hydrogen, carbon monoxide and carbon dioxide at a pressure of 50-100 atm and 250 – 300°C in the presence of copper catalyst (low pressure process). The process generally consists of four steps:

1. Pretreatment of feedstock for removal of sulphur.
2. Steam reforming for production of synthesis gas, sulphur free natural gas mixed with three volumes of steam are reformed at 815 – 843°C in presence of nickel oxide catalyst.
3. Methanol synthesis is conducted in methanol converter at about 250°C and 100 atm in the presence of copper catalyst.
4. The methanol formed is purified in a number of distillation columns one, two, three depending on end use. The production of methanol from coal involves gasification of coal, followed by shift reaction for generating synthesis gas with H_2/CO ratio of 2:1. The synthesis gas is subsequently converted like natural gas.

5.1 Production Methods

The by far dominating production method of methanol synthesis is through the synthesis gas process first developed during the 1920s. A gas mixture of hydrogen and carbon monoxide (usually also carbon dioxide), known as synthesis gas (syngas) is the basis for almost all methanol production today.

5.1.1 Methanol synthesis with Syn Gas

The production of methanol usually consists of three basic steps independent of feed-stock material: synthesis gas preparation, methanol synthesis and methanol purification. In order to properly understand the challenges of different processes to produce the synthesis gas, we first need to understand the process from synthesis gas to methanol, the methanol synthesis. In essence the process consists of the three following equations:



All three equations are reversible and thus the process conditions regarding temperature, pressure and synthesis gas mixture are important to control. It can also be noted that equation (1) and (2) are exothermic, i.e. the processes produce heat and require cooling. Some heat is normally recovered and used for other parts of the synthesis.

While it was originally believed that the main process that produce methanol was the reaction between carbon monoxide and hydrogen (equation 1) it is now understood that carbon dioxide is just as important in the synthesis process. CO_2 even used to be scrubbed from the reactant mixture but a scrubber failure at Imperial Chemical Industries (ICI) with a resulting increase of methanol production showed that CO_2 was active and important in the reaction. Subsequent studies have shown that it is mainly the CO_2 that is converted to methanol while CO acts as a reducing agent for oxygen at the surface of the catalyst.

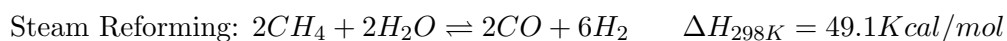
Equation (3) describes the reverse water gas shift reaction that produces carbon monoxide from carbon dioxide and hydrogen. The carbon monoxide then reacts with hydrogen to produce methanol (equation 2). Equation 2 is actually merely the sum of (1) and (3). To synthesize methanol, a specific H_2/CO ratio of 2 in the synthesized gas is required. Temperature is kept around $580 - 600^\circ C$ and Pressure 300-600 KPa.

5.1.2 Synthesis gas production from Natural Gas

Before natural gas is processed to synthesis gas impurities need to be removed. The most important are sulphur compounds (such as H_2S) because of the poisonous effects these have on catalysts downstream. Other impurities such as carbon dioxide, nitrogen and oxygen.

5.1.2.1 Steam Methane Reforming

The traditionally dominating method is through steam reforming where methane gas and steam is mixed at high temperature and pressure and with the help of catalysts form carbon monoxide and hydrogen (Equation 4). The gas mixture is typically led through pipes coated with catalysts in a tube in shell heat exchanger in order to provide the necessary heat ($850^\circ C$) for the reaction to take place.



Carbon dioxide is typically added to the gas mixture before the methanol synthesis but can also be present in the natural gas used as feedstock.

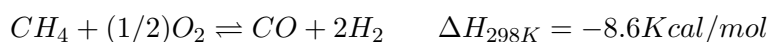
Remembering that the H_2/CO ratio should be 2 for methanol synthesis we observe that steam reforming produces an excess of hydrogen which needs to be subtracted and is usually burnt to provide heat for the reformation to take place but can also be used for other purposes. The synthesis gas production is strongly endothermic and requires a lot of thermal energy. The methanol synthesis produce some heat that can be recovered but

heat is normally also provided by burning a portion of the natural gas. The synthesis gas production and subsequent compression stands for a large amount of the investment cost in a methanol production plant and most of the energy need to power the process and represents as much as 60 % of the capital cost.

One step reforming through steam reforming used to be the dominating process but is today mainly considered for smaller plants up to 2500 MTPD where CO_2 is available at low cost or contained in the natural gas.

5.1.2.2 Partial Oxidation

Another basic route for synthesis gas production is partial oxidation. Originally developed by Shell in the 1950s.



The partial oxidation process for methane is slightly exothermic. The process occurs in the gas phase via radical reaction within the flame of the burner. A small excess of oxygen is needed to favor some oxidation to carbon dioxide and water in order to bring up the temperature to the desired 1000 – 1200°C, unfortunately that produces carbon dioxide and water that lowers the stoichiometric number to about 1.6 which is below the preferred 2 but an improvement over steam reforming.

A large cost for a partial oxidation plant is the air separator needed to produce oxygen. While it is possible to use air most modern plants use pure oxygen to avoid the need of separating mainly nitrogen from the synthesis gas after the oxidation step.

5.1.2.3 Two-step Reforming

A combination of steam reforming and partial oxidation offers a mean to improve the overall process and to better control the composition of the produced synthesis gas. The right system configuration depends on the composition of the natural gas used as feedstock. Two step reforming also requires that the steam reforming operates with high methane slip, usually 35-45 %, to provide a high enough methane content for the partial oxidation step.

The technique is fairly new and was first used in a 2400 MTPD commercial plant in Norway 2007 and a 5000 MTPD plant with similar technology in Saudi Arabia 2008.

5.1.2.4 Dry Reforming

By reacting methane and carbon dioxide synthesis gas is produced in a process called dry reforming as no steam is used.



The reaction is more endothermic than steam reforming and produces a gas with significant hydrogen deficit for methanol synthesis. While this is a disadvantage for methanol synthesis the gas mixture has the right composition for other applications.

5.1.2.5 Synthesis Gas from Coal

The process to convert coal to synthesis gas is a combination of partial oxidation and steam treatment called gasification.



The design and processing conditions vary greatly depending on the composition of the coal used as feedstock. The synthesis gas produced have a deficit of hydrogen and must be subjected to the water gas shift reaction (equation 12) in improve the H_2/CO ratio. The synthesis gas produced from coal is usually in higher need of purification than that produced from natural gas, especially sulphur compounds must be removed before the methanol synthesis to protect the sensitive catalysts from poisoning.

5.1.2.6 Biomass

In contrast to ethanol, methanol can rather easily be produced from virtually all biomass such as wood, algae, agricultural waste and municipal waste through gasification. Production from biomass does however offer challenges that need to be addressed especially regarding the cost of production. Due to the composition of biomass the production plants inquire high capital investment costs and has lower energy conversion efficiency compared to natural gas and coal.

The conventional method to produce methanol from biomass is through gasification of the feedstock material. An attractive alternative is enzymatic conversion, although most research in this area is currently focused on ethanol production.

Another alternative mainly for sea growing plants like macro and micro-algae as well as water hyacinth and cattail etc. is anaerobic digestion that produces methane that could be used in the same way as natural gas. As with enzymatic conversion the methods is still in need of further research and development before large scale commercial implementation is possible.

The gasification process of biomass is similar to the synthesis gas process from coal. For gasification of biomass the feedstock is first dried and pulverized. The moist content should generally be no higher than 15-20 wt%. The first step in a two-step gasification process is called Pyrolysis, or destructive distillation. The dried biomass is heated to 400 – 600°C in an oxygen deficient environment to prevent complete combustion. Carbon monoxide, carbon dioxide, hydrogen, methane as well as water and volatile tars are released. The remaining biomass (10-25 wt%), called charcoal, is further reacted with oxygen at high temperature (1300 – 1500°C) to produce mainly carbon monoxide.

The synthesis gas produced from the pyrolysis and charcoal conversion is purified before the methanol synthesis. Compared to coal biomass consists of much less sulphur but the tar content offers operational challenges as it condense easily in pipes, filters and boilers. This can to an extent be controlled by choosing the right operational pattern and technique according to the composition of the available biomass. A one step partial oxidation process is an attractive alternative but the technical challenges have so far prevented large scale operation.

Production from biomass is possible at small scale but as with natural gas and coal large scale production is preferred due to the high system costs. The logistical challenges for a biomass plant are however great due to the lower energy content in biomass compared

to natural gas and coal implying a large demand of feedstock material.

The quantities needed to feed a 2500 MTPD plant is estimated to 1.5 million ton biomass per year with put large strains on collection, transportation and storage of biomass and might be one of the largest hurdles towards the construction on mega sized plants.

5.1.3 Black Liquor from Pulp

Black liquor from the pulp industry has been identified as an interesting feedstock for renewable energy. Black liquor is formed as pulpwood is mixed with chemicals (white liquor) to produce pulp as a pre stage to paper production. Black liquor can be gasified and used for methanol synthesis. The chemicals are recovered and reused.

Black liquor is available in large quantities worldwide and offers a feasible way to produce methanol. An industrial scale demonstration plant at the Smurfit Kappa paper mill in Pite, Sweden has been operational since 2010 producing DME.



5.2 Methanol Purification

Regardless of the synthesis method the crude methanol produced contains impurities to a smaller or larger degree. The largest impurity is usually water which can be as much as 18 %. The first stage in a common two-step purification process is to remove the low boiling purifications, typically called light ends. This is done in a topping column where the low boiling compounds are boiled off to produce a mixture of methanol and water. A refining column is used to separate water and methanol under heavy boiling. The refining column needs to be high as methanol and water is reluctant to separate easily. Good quality methanol eventually accumulates in the top of the column and is transferred to a storage tank. Water accumulates in the bottom and taken to a treatment facility before disposal.

Chapter 6

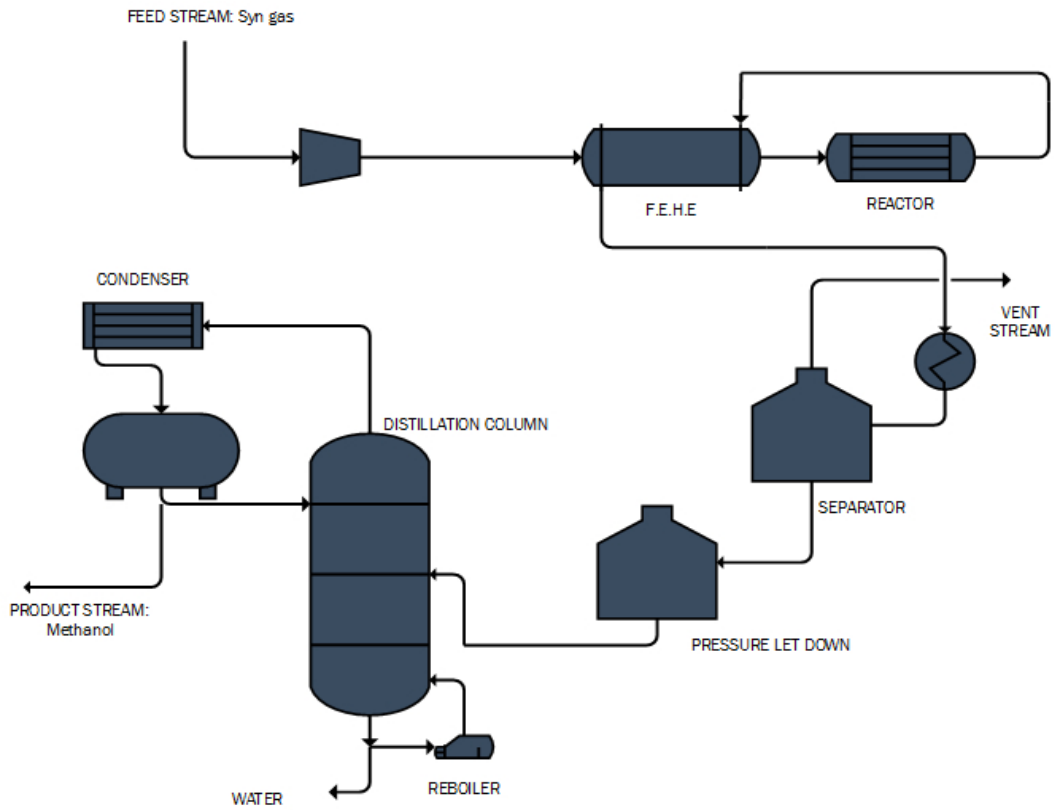
Process Selection and Description

Syngas comprising of CO , CO_2 , CH_4 , H_2 , H_2O is compressed to very high pressures (depending on the catalyst used by the process licensor). In this process, the syngas is compressed to 110 bar of pressure. This stream along with three other recycled streams enter a Feed-Effluent Heat Exchanger (FEHE) in which it is heated to about $150^\circ C$.

This stream enters a tubular reactor comprising of $Cu/Zn/Al_2O_3$ based catalyst (void fraction 0.5) in which the exothermic reaction takes place thus producing Methanol. The stream exiting from the reactor comprises of Methanol along with the unreacted gas at a temperature of $267^\circ C$ and pressure of approximately 107 bar (considering 3 bar pressure drop).

This stream is cooled in the FEHE thus preheating the incoming stream. This stream from the reactor is being cooled down to $175^\circ C$ and is again sent to an exchanger. It is again sent to an exchanger where it is partially condensed at constant pressure at around $38^\circ C$. Some of the vapours are vented out to prevent the built up of inerts. The stream from the high pressure separator is flashed into a flash tank at constant temperature and the pressure is reduced to 2 bar.

The product stream moves from flash tank to the distillation column with the help of a centrifugal pump. The flow rate of the stream to the distillation column is regulated by a control valve. The column operates at 1 bar pressure. A small vapour stream from the top of the reflux drum recycles the small amount of inert components entering the column. This small vapour stream is then compressed back to 110 bar and is recycled

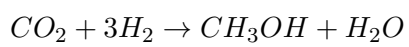
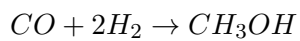


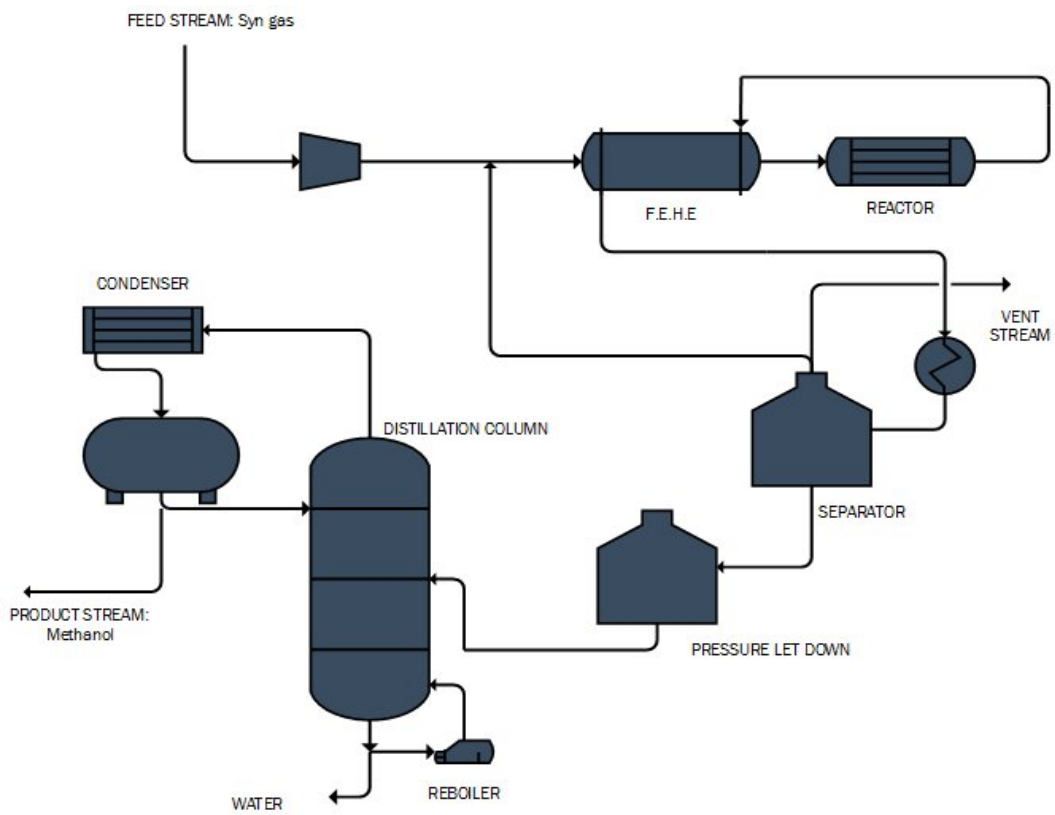
PROCEES FLOW DIAGRAM: Without Recycle

FIGURE 6.1: Process Flow Diagram (Without Recycle)

THE NATION BUILDERS UNIVERSITY

back to the feed stream. The final product from the column is methanol and water is obtained as the bottom product.





PROCEES FLOW DIAGRAM: Without Recycle

FIGURE 6.2: Process Flow Diagram (With Recycle)

Chapter 7

Calculations

7.1 Mass Balance

Feed requirement for 400 TPD of product methanol (with and without recycle):

Distillation Column:

Specifications

Percentage separation of column = 99.9%

0.1mol% of H_2O in feed goes into distillate

0.1mol% of methanol in feed goes to bottoms

400 TPD of methanol = $\frac{4 \times 10^5}{24 \times 32} = 520.83$ Kmol/hr (output of distillation column in top product)

Applying material balance:

$0.999 X = 520.83$ (Considering 99.9% separation)

$X = 521.35$ Kmol/hr

X is the methanol present in the feed to the distillation column.

Total water in the stream = Water in the feed + Water in the reactor

= $38.48 + 3.28037 = 41.76$ Kmol/ hr

Water in the top product = 0.042 Kmol/ hr

Water in the bottoms = 41.72 Kmol/ hr

Methanol in bottoms = 0.52 Kmol/ hr

TOP:

$$CH_3OH = 520.83 \text{ Kmol/hr}$$

$$H_2O = 0.042 \text{ Kmol/hr}$$

BOTTOM:

$$CH_3OH = 0.52 \text{ Kmol/hr}$$

$$H_2O = 41.7 \text{ Kmol/hr}$$

Reactor:



Feed composition obtained from **industrial data:**

On mole fraction basis:

$$H_2 \rightarrow 0.675$$

$$N_2 \rightarrow 0.003$$

$$CO \rightarrow 0.23$$

$$CO_2 \rightarrow 0.069$$

$$CH_4 \rightarrow 0.022$$

$$H_2O \rightarrow 0.001$$



Let total feed amount entering in the reactor be **yKmol/hr**.

According to first reaction:

1 mole of CO will produce 0.64 moles of CH_3OH

0.23y moles of CO will produce $0.64 \times 0.23y$ moles of CH_3OH

According to second reaction:

1 mole of CO_2 will produce 0.17 moles of CH_3OH

0.069y moles of CO_2 will produce $0.17 \times 0.069y$ moles of CH_3OH

Now,

Total moles of CH_3OH produced by both reactions should be equal to CH_3OH entering in the distillation column

$$(0.64 \times 0.23y) + (0.17 \times 0.069y) = 521.35$$

$$y = 3280.37 \text{ Kmol/hr}$$

Hence the feed entering in the reactor is 3280.37 Kmol/hr.

Now, calculating composition of each component entering in the reactor,

$$\text{CO} = 0.23 \times 3280.37 = 754.48 \text{ Kmol/hr}$$

$$\text{CO}_2 = 0.069 \times 3280.37 = 226.34 \text{ Kmol/hr}$$

$$\text{H}_2 = 0.675 \times 3280.37 = 2214.24 \text{ Kmol/hr}$$

$$\text{CH}_4 = 0.022 \times 3280.37 = 72.17 \text{ Kmol/hr}$$

$$\text{H}_2\text{O} = 0.001 \times 3280.37 = 3.28037 \text{ Kmol/hr}$$

$$\text{N}_2 = 0.003 \times 3280.37 = 9.8411 \text{ Kmol/hr}$$

$$\text{Amount of CO reacted} = 754.48 \times 0.64 = 482.87 \text{ Kmol/hr}$$

$$\text{Amount of CO}_2 \text{ reacted} = 226.34 \times 0.17 = 38.48 \text{ Kmol/hr}$$

$$\text{Amount of H}_2 \text{ reacted} = (2 \times 482.87) + (3 \times 38.48) = 1081.18 \text{ Kmol/hr}$$

$$\text{Amount of CO unreacted} = 754.48 - 482.87 = 271.61 \text{ Kmol/hr}$$

$$\text{Amount of CO}_2 \text{ unreacted} = 226.34 - 38.48 = 187.86 \text{ Kmol/hr}$$

$$\text{Amount of H}_2 \text{ unreacted} = 2214.24 - 1081.18 = 1133.06 \text{ Kmol/hr}$$

SEPARATOR:

Input to separator:

$$\text{CH}_3\text{OH} = 521.35 \text{ Kmol/hr}$$

$$\text{H}_2\text{O} = 41.76 \text{ Kmol/hr}$$

$$\text{CO} = 271.61 \text{ Kmol/hr}$$

$$\text{CO}_2 = 187.86 \text{ Kmol/hr}$$

$$\text{H}_2 = 1133.06 \text{ Kmol/hr}$$

$$\text{CH}_4 = 72.17 \text{ Kmol/hr}$$

$$\text{N}_2 = 9.841 \text{ Kmol/hr}$$

Vent Specifications:

0.022 of non-condensable gases is vented out.

Vented stream composition

$$\text{CO} = 5.97 \text{ Kmol/hr}$$

$$CO_2 = 4.13 \text{ Kmol/hr}$$

$$H_2 = 24.92 \text{ Kmol/hr}$$

$$N_2 = 0.918 \text{ Kmol/hr}$$

$$CH_4 = 1.58 \text{ Kmol/hr}$$

Recycle stream (R) = Separator feed – Vent stream

Recycle stream Composition

$$CO = 265.63 \text{ Kmol/hr}$$

$$CO_2 = 183.72 \text{ Kmol/hr}$$

$$H_2 = 1108.14 \text{ Kmol/hr}$$

$$CH_4 = 70.58 \text{ Kmol/hr}$$

$$N_2 = 8.92 \text{ Kmol/hr}$$

Specified Feed after Recycle:

$$CO = 754.48 - 265.635 = 488.84 \text{ Kmol/hr}$$

$$CO_2 = 226.34 - 183.729 = 42.61 \text{ Kmol/hr}$$

$$H_2 = 2214.24 - 1108.14 = 1106.1 \text{ Kmol/hr}$$

$$CH_4 = 72.17 - 70.583 = 1.59 \text{ Kmol/hr}$$

$$N_2 = 9.84 - 8.92 = 0.92 \text{ Kmol/hr}$$

$$H_2O = 3.28 - 0 = 3.28 \text{ Kmol/hr}$$

Total feed flow rate = 1683.34 Kmol/hr.

7.2 Heat Balance

C_P values for gases:

$$CO = 6.6 + 0.0012T$$

$$CO_2 = 10.34 + 0.00274T - 195500/T^2$$

$$H_2 = 6.62 + 0.00081T$$

$$H_2O = 8.22 + 0.00015T + 0.00000134T^2$$

$$N_2 = 6.5 + 0.001T$$

$$CH_4 = 5.34 + 0.0115T$$

Component	C_P Value, cal/mol K	Molar Flow Rate, Kmol/hr	X_i	$X_i C_{Pi}$
CO	6.987	488.84	0.290	2.03
CO ₂	9.351	82.611	0.049	0.46
H ₂	6.88	1106.1	0.657	4.52
H ₂ O	8.408	3.28	0.002	0.02
N ₂	6.823	0.92	0.001	0.00
CH ₄	9.054	1.59	0.001	0.01
		1683.341		7.037

TABLE 7.1: Feed Stream Composition

Calculations for Real gases:

For Compressor:

$$\Delta T = \frac{T_1 [P_2/P_1]^{(k-1)/k} - 1}{\eta}$$

$$T_2 = T_1 + \Delta T$$

$$T_1 = 323K, P_1 = 51bar, P_2 = 110bar, T_2 = 401K$$

Using SRK Equation:

$$P = \frac{RT}{V-b} - \frac{a}{\sqrt{TV}(V+b)}$$

or

$$V^3 - \frac{RT(V^2+Vb)}{P} + \frac{(b^2-a)V}{P\sqrt{T}} = \frac{ab}{P\sqrt{T}}$$

Finding the constant a and b:

$$a = \frac{0.4278R^2T_C^{2.5}}{P_C}$$

$$b = \frac{0.0867RT_C}{P_C}$$

For CO:

$$T_C = 132.86K$$

$$P_C = 35bar$$

$$a = \frac{0.4278 \times 8.314^2 \times 132.86^{2.5}}{35}$$

$$a = 169132.7 Nm^4 K^{0.5} / mol$$

$$b = \frac{0.0867 \times 8.314 \times 132.86}{35}$$

$$b = 2.736 m^3 / mol$$

For H_2 :

$$T_C = 33.16K$$

$$P_C = 13bar$$

$$a = \frac{0.4278 \times 8.314^2 \times 33.16^{2.5}}{13}$$

$$a = 14403.02 Nm^4 K^{0.5} / mol$$

$$b = \frac{0.0867 \times 8.314 \times 33.16}{13}$$

$$b = 1.838 m^3 / mol$$

For CO_2 :

$$T_C = 305K$$

$$P_C = 73.8bar$$

$$a = \frac{0.4278 \times 8.314^2 \times 305^{2.5}}{73.8}$$

$$a = 650959.63 Nm^4 K^{0.5} / mol$$

$$b = \frac{0.0867 \times 8.314 \times 305}{73.8}$$

$$b = 2.97 m^3 / mol$$

For the mixture:



$$\begin{aligned} a_{mix} &= x_{CO} \times a_{CO} + x_{H_2} \times a_{H_2} + x_{CO_2} \times a_{CO_2} \\ &= 0.236 \times 169132.7 + 0.693 \times 14403.02 + 0.07 \times 650959.63 \\ &= 95463.78 Nm^4 K^{0.5} / mol \end{aligned}$$

$$\begin{aligned} b_{mix} &= x_{CO} \times b_{CO} + x_{H_2} \times b_{H_2} + x_{CO_2} \times b_{CO_2} \\ &= 0.236 \times 2.736 + 0.693 \times 1.838 + 0.07 \times 2.97 \\ &= 2.127 m^3 / mol \end{aligned}$$

In the stream,

$$P = 51 \text{ bar}$$

$$T = 323 \text{ K}$$

Substituting these values in the SRK equation, we get:

$$V^3 - 52.655V^2 - 7.84V - 221.53 = 0$$

We get one of the roots as:

$$V = 52.88m^3$$

Total molar flow rate = 1683.341 Kmol/hr.

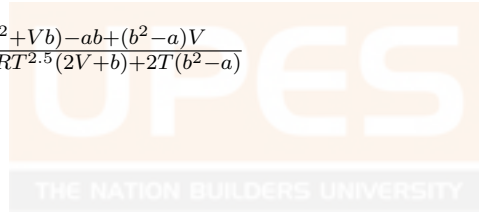
Differentiating the SRK equation with respect to temperature at **constant pressure**:

$$V^3 - \frac{RT(V^2+Vb)}{P} + \frac{(b^2-a)V}{P\sqrt{T}} = \frac{ab}{P\sqrt{T}}$$

$$3V^2\left(\frac{\delta V}{\delta T}\right)_P - \frac{RT(2V+b)}{P}\left(\frac{\delta V}{\delta T}\right)_P - \frac{R(V^2+Vb)}{P} + \frac{(b^2-a)}{P\sqrt{T}}\left(\frac{\delta V}{\delta T}\right)_P - \frac{(b^2-a)V}{2PT^{1.5}} = -\frac{ab}{2PT^{1.5}}$$

$$\left(\frac{\delta V}{\delta T}\right)_P \left[\frac{3P\sqrt{T}V^2 + b^2 - a + RT^{1.5}(2V+b)}{P\sqrt{T}} \right] = \frac{RT^{1.5}(V^2+Vb) - ab + (b^2-a)V}{PT^{1.5}}$$

$$\left(\frac{\delta V}{\delta T}\right)_P = \frac{2RT^{1.5}(V^2+Vb) - ab + (b^2-a)V}{6PV^2T^{1.5} - 2RT^{2.5}(2V+b) + 2T(b^2-a)}$$



Putting the values in the above equation, we get:

$$\left(\frac{\delta V}{\delta T}\right)_P = 0.1786 m^3/K$$

Now similarly, differentiating the SRK equation with respect to pressure at constant temperature:

$$V^3 - \frac{RT(V^2+Vb)}{P} + \frac{(b^2-a)V}{P\sqrt{T}} = \frac{ab}{P\sqrt{T}}$$

$$3V^2\left(\frac{\delta V}{\delta P}\right)_T - \frac{RT(2V+b)}{P}\left(\frac{\delta V}{\delta P}\right)_T + \frac{RT(V^2+Vb)}{P^2} + \frac{(b^2-a)}{P\sqrt{T}}\left(\frac{\delta V}{\delta P}\right)_T - \frac{(b^2-a)V}{P^2\sqrt{T}} = -\frac{ab}{P^2\sqrt{T}}$$

$$\left(\frac{\delta V}{\delta P}\right)_T \left[\frac{3PV^2\sqrt{T} - RT^{1.5}(2V+b) + (b^2-a)}{P\sqrt{T}} \right] = \frac{(b^2-a)V - ba - RT^{1.5}(V^2+Vb)}{P^2\sqrt{T}}$$

$$\left(\frac{\delta V}{\delta P}\right)_T = \frac{(b^2-a)V - ba - RT^{1.5}(V^2+Vb)}{3P^2V^2\sqrt{T} - PRT^{1.5}(2V+b) + (b^2-a)P}$$

$$\left(\frac{\delta V}{\delta P}\right)_T = -1.196 \text{ m}^3/\text{bar}$$

Since we know that,

$$\begin{aligned}\beta &= \frac{1}{V} \left(\frac{\delta V}{\delta T}\right)_P \\ &= 0.0038 \text{ K}^{-1}\end{aligned}$$

$$\begin{aligned}\kappa &= -\frac{1}{V} \left(\frac{\delta V}{\delta P}\right)_T \\ &= 0.022 \text{ bar}^{-1}\end{aligned}$$

$$\begin{aligned}C_P - C_V &= \frac{\beta^2 V T}{\kappa} \\ &= 8.869 \text{ bar m}^3/\text{K}\end{aligned}$$

$$C_P = 29.418 \frac{\text{KJ}}{\text{KmolK}}$$

$$C_V = 29.418 - 8.869$$

$$C_V = 20.549 \frac{\text{KJ}}{\text{KmolK}}$$

$$\begin{aligned}\gamma &= \frac{C_P}{C_V} \\ &= \frac{29.418}{20.549} \\ &= 1.43\end{aligned}$$



Energy Balance of Feed stream:

$$H = \int_{298}^{401} (CO + CO_2 + H_2 + H_2O + N_2 + CH_4) dT$$

- $CO = \int_{298}^{401} m C_p dT$
 $= \int_{298}^{401} 448.84 \times (6.6 + 0.0012T) dT$
 $= 448.84 [3226.34T + 0.2933T^2]$
 $= 353430.44 \text{ Kcal/hr}$

- $CO_2 = \int_{298}^{401} m C_p dT$
 $= \int_{298}^{401} 82.611 \times (10.34 + 0.00274T - 195500/T^2) dT$
 $= 82.611 [10.34T + 0.00137T^2 + 195500/T]_{298}^{401}$

$$= 82210.001 \text{ Kcal/hr}$$

$$\begin{aligned} \bullet H_2 &= \int_{298}^{401} mC_p dT \\ &= \int_{298}^{401} 1106.1 (6.62 + 0.00081T) dT \\ &= 786457.878 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet H_2O &= \int_{298}^{401} mC_p dT \\ &= \int_{298}^{401} 3.28 (8.22 + 0.00015T + 0.00000134T^2) dT \\ &= 2850.446 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet N_2 &= \int_{298}^{401} mC_p dT \\ &= \int_{298}^{401} 0.92 (6.5 + 0.001T) dT \\ &= 649.058 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CH_4 &= \int_{298}^{401} mC_p dT \\ &= \int_{298}^{401} 1.59 (5.34 + 0.0115T) dT \\ &= 1532.764 \text{ Kcal/hr} \end{aligned}$$

$$\sum(CO + CO_2 + H_2 + H_2O + N_2 + CH_4) = 1227130.657 \text{ Kcal/hr.}$$

Recycle Stream:

Component	C_P Value, cal/mol K	Molar Flow Rate, Kmol/hr	X_i	$X_i C_{Pi}$
CO	6.973	265.635	0.16	1.130
CO ₂	9.17	183.729	0.11	1.03
H ₂	6.871	1108.14	0.68	4.652
H ₂ O	0	0	0	0
N ₂	6.811	8.923	0.01	0.034
CH ₄	8.916	70.58	0.04	0.383
		1637.01		7.226

TABLE 7.2: Recycle Stream Composition

Energy balance for Recycle stream:

$$H = \int_{298}^{311} CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$\begin{aligned} \bullet CO &= \int_{298}^{311} mC_p dT \\ &= \int_{298}^{311} 265.635 \times (6.6 + 0.0012T) dT \\ &= 265.635 [1753.191T + 0.159T^2]_{298}^{311} \\ &= 24053.30 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CO_2 &= \int_{298}^{311} mC_p dT \\ &= \int_{298}^{311} 183.729 \times (10.34 + 0.00274T - 195500/T^2) dT \\ &= 183.729 [10.34T + 0.00137T^2 + 195500/T]_{298}^{311} \\ &= 21651.247 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet H_2 &= \int_{298}^{311} mC_p dT \\ &= \int_{298}^{311} 1108.14 (6.62 + 0.00081T) dT \\ &= 98919.651 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet N_2 &= \int_{298}^{311} mC_p dT \\ &= \int_{298}^{311} 8.923 (6.5 + 0.001T) dT \\ &= 789.315 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CH_4 &= \int_{298}^{311} mC_p dT \\ &= \int_{298}^{311} 70.583 (5.34 + 0.0115T) dT \\ &= 8113.004 \text{ Kcal/hr} \end{aligned}$$

$$\Sigma(CO + CO_2 + H_2 + H_2O + N_2 + CH_4) = 153526.517 \text{ Kcal/hr}$$

Mixing: Feed stream+ Recycle stream

$$= \text{Feed energy} + \text{recycle energy} = 1227130.657 + 153526.517$$

$$= 1380657.174 \text{ Kcal/hr.}$$

$$H_m = \int_{298}^T CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$= \triangleright 22868.102T + 2.134T^2 + 0.000001464T^3 + 52069470/T = 1380657.174$$

$$T = 356^\circ K = 83^\circ C$$

Calculations for Reactor:

$$H = \int_{298}^{540} CO + CO_2 + H_2 + H_2O + N_2 + CH_4 + CH_3OH dT$$

$$\begin{aligned} \bullet CO &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 271.61 \times (6.6 + 0.0012T) dT \\ &= 271.61[6.6T + 0.0006T^2] \\ &= 466847.156 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CO_2 &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 187.86 (10.34 + 0.00274T - 195500/T^2) dT \\ &= 187.86 [10.34T + 0.00137T^2 + 195500/T] \\ &= 467040.115 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet H_2 &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 1133.06 (6.62 + 0.00081T) dT \\ &= 1908268.357 \text{ Kcal/hr.} \end{aligned}$$

$$\begin{aligned} \bullet H_2O &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 41.76 (8.22 + 0.00015T + 0.00000134T^2) dT \end{aligned}$$

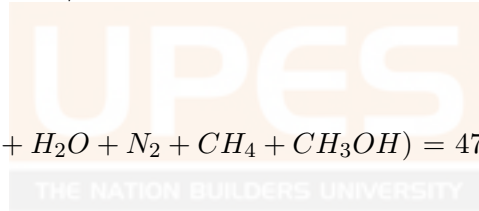
$$= 86148.979 \text{ Kcal/hr}$$

$$\begin{aligned} \bullet N_2 &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 9.841 (6.5 + 0.001T) dT \\ &= 16477.918 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CH_4 &= \int_{298}^{540} mC_p dT \\ &= \int_{298}^{540} 72.17 (5.34 + 0.0115T) dT \\ &= 177419.624 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} \bullet CH_3OH &= \int_{298}^{540} mC_p dT \\ &= 521.35 \times 3084.03 \\ &= 1607859.162 \text{ Kcal/hr} \end{aligned}$$

$$\Sigma(CO + CO_2 + H_2 + H_2O + N_2 + CH_4 + CH_3OH) = 47300061.311 \text{ Kcal/hr.}$$



Calculations for X:

$$H_X = \int_{298}^{448} CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$\begin{aligned} \bullet CO &= \int_{298}^{448} mC_p dT \\ &= \int_{298}^{448} 271.61 \times (6.6 + 0.0012T) dT \end{aligned}$$

$$\begin{aligned} \bullet CO_2 &= \int_{298}^{448} mC_p dT \\ &= \int_{298}^{448} 187.86 (10.34 + 0.00274T - 195500/T^2) dT \end{aligned}$$

$$\begin{aligned} \bullet H_2 &= \int_{298}^{448} mC_p dT \\ &= \int_{298}^{448} 1133.06 (6.62 + 0.00081T) dT \end{aligned}$$

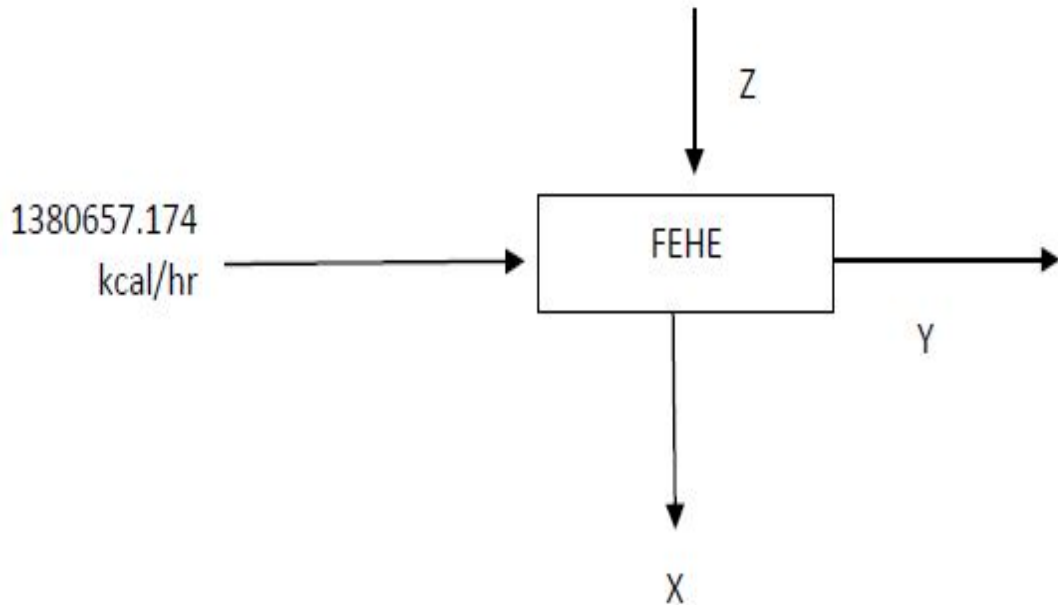


FIGURE 7.1: F.E.H.E. Flow diagram

$$\bullet H_2O = \int_{298}^{448} mC_p dT$$

$$= \int_{298}^{448} 41.76 (8.22 + 0.00015T + 0.00000134T^2) dT$$

$$\bullet N_2 = \int_{298}^{448} mC_p dT$$

$$= \int_{298}^{448} 9.841 (6.5 + 0.001T) dT$$

$$\bullet CH_4 = \int_{298}^{448} mC_p dT$$

$$= \int_{298}^{448} 72.17 (5.34 + 0.0115T) dT$$

$$\sum(CO+CO_2+H_2+H_2O+N_2+CH_4) = [12028.58T + 1.302T^2 + 0.0000186T^3 + 36726630/T]_{298}^{448}$$

$$= 1909894.863 \text{ Kcal/hr}$$

Calculations for liquid Methanol:

$$CH_3OH = \int_{298}^{448} mC_p dT$$

$$\begin{aligned} & [521.35 (105800T - 181.115T^2 + 0.3126T^3)]_{298}^{448} \\ & = 1925535.653 \text{ Kcal/hr} \end{aligned}$$

$$\begin{aligned} X &= \sum(CO + CO_2 + H_2 + H_2O + N_2 + CH_4 + \text{liquid Methanol}) \\ &= 1909894.863 + 1925535.653 = 3835430.516 \text{ Kcal/hr.} \end{aligned}$$

Calculations for Z:

Output reactor heat + latent heat of methanol

$$\text{Reactor output heat} = 47300061.311 \text{ kcal/hr}$$

Now,

Calculation for latent heat of methanol:

$$\text{Latent heat} = \Delta H_r = C_1 \times (1 - T_r)^{C_2 + C_3 \times T_r + C_4 \times T_r^2}$$

$$T_r = \frac{T_{sat}}{T_c}$$

From the above flow rate table:

$$x_{CH_3OH} = 521.35 / 2237.6511$$

$$= 0.2329$$

$$x_{H_2O} = 41.76 / 2237.6511$$

$$= 0.0186$$

$$P_{CH_3OH} = x \times P_T$$

$$= 0.2329 \times 82500$$

$$= 25.62 \text{ mmHg}$$

$$P_T = 110 \text{ bar} = 82500 \text{ mmHg}$$

Antoine Equation:

$$\log P^{vap} = A - \frac{B}{C+T}$$

$$A = 7.87863, B = 1473.11, C = 230$$

$$\log 19214.25 = 7.87863 - \frac{1473.11}{230+T}$$

$$T = 179.76^\circ C = 452.76^\circ K$$

$$T_r = \frac{T_{sat}}{T_c}$$

$$T_c(CH_3OH) = 512.64^\circ K$$

$$T_r = 0.882$$

$$C_1(\text{methanol}) = 5.239 \times 10^7$$

$$C_2(\text{methanol}) = 0.3682$$

Substituting values in Antoine Equation :

$$L = (5.239 \times 10^7)(1 - 0.882)^{0.3682} = 5693.864 \text{ Kcal}$$

$$L = 56693.864 \text{ Kcal/hr}$$

$$H_L = \text{mL}$$

$$H_L = 521.35 \times 5693.864$$

$$H_L = 2968496.275 \text{ Kcal}$$

Z = Output reactor heat + latent heat of methanol

$$Z = 4730061.311 + 2968496.275$$

$$Z = 7698557.586 \text{ Kcal/hr}$$

Calculations for Y:

Applying,

Heat in = Heat out (for FEHE)

Feed in + Z = X + Y

$$1380657.174 + 7698557.586 = 3835430.516 + Y$$

$$Y = 5243784.244 \text{ Kcal/hr}$$

Calculation for energy of stream Y:

$$H_Y = \int_{298}^T CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$H_Y = 5243784.244 \text{ Kcal/hr}$$

$$5243784.24 = \int_{298}^T CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$5243784.244 = [22868.102T + 2.134T^2 + 0.00001464T^3 + 52069470/T]_{298}^T$$

$$T = 514^\circ K = 241^\circ C$$

Now coming on to heat exchanger before separator:

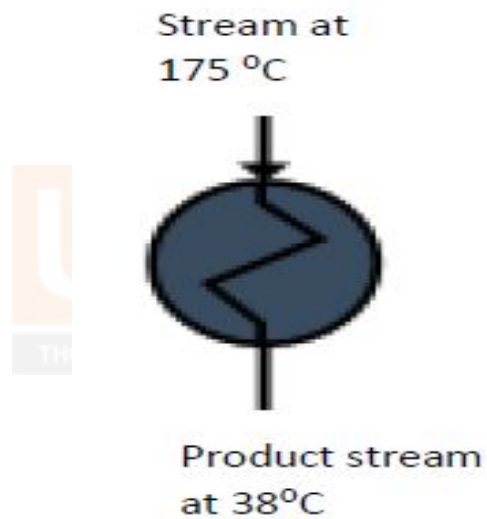


FIGURE 7.2: Heat Exchanger 2

Calculation for latent heat of water

$$T_r = \frac{T_{sat}}{T_c}$$

$$T_C(H_2O) = 647.13K$$

$$T_r = 0.882$$

$$C_1(H_2O) = 5.2053 \times 10^7$$

$$C_2(H_2O) = 0.3199$$

$$C_3(H_2O) = -0.212$$

$$C_4(H_2O) = 0.25795$$

Substituting all these in Antoine Equation:

$$L = (5.2053 \times 10^7)(1 - 0.608)^{0.3199 + (-0.212)0.608 + 0.25795(0.608)^2}$$

$$L = 39797.83888 \text{ KJ/ kmol} - K$$

$$H_{Lw} = mL$$

$$= 41.76(39797.838)$$

$$= 1661957.75 \text{ KJ/hr}$$

$$= 397597.54 \text{ kcal/hr}$$



Energy of stream at $175^{\circ}C = X + H_w$

$$= 3835430.516 + 397597.54 = 4233028.064 \text{ Kcal/hr}$$

Calculations for liquid H_2O :

$$H(H_2O) = \int_{298}^{311} mC_p dT$$

$$= 41.76(74.802)(311 - 298)$$

$$= 40608.50 \text{ KJ/hr}$$

$$= 9714.952 \text{ kcal/hr}$$

Energy of gases at $38^{\circ}C$:

$$H_g = \int_{298}^{311} CO + CO_2 + H_2 + H_2O + N_2 + CH_4 dT$$

$$= (116853.1T + 1.299T^2 + \frac{36726630}{T})_{298}^{311}$$

$$= 157041.546 \text{ kcal/hr}$$

Energy of liquid methanol at 38°C :

$$CH_3OH = \int_{298}^{311} mC_p dT$$

$$[521.35 (105800T - 181.115T^2 + 0.3126T^3)]_{298}^{311}$$

$$= 133729.1 \text{ Kcal/hr}$$

Energy of stream at 38°C = energy of gases + energy of liquid H_2O + energy of liquid methanol

$$= 157041.546 + 9714.952 + 133729.1$$

$$= 2092292.151 \text{ Kcal/hr}$$

$$\text{Heat lost in heat exchanger} = \text{energy of products at } 175^\circ\text{C} - \text{energy of products at } 38^\circ\text{C}$$

$$= 4233028.064 - 2092292.157$$

$$= 2140735.913$$



7.3 Distillation Column

Selection of Operating Pressure:

The operating pressure has been selected as 1 atm as it cannot be operated below 1 atm as the latent heat of condensation will be higher as the saturation pressure is reduced. The driving force, as a rule of thumb should be at least and in this case it is around $32^{\circ}C$ assuming coolant water is at $32^{\circ}C$.

Degree of Separation:

Since methanol water separation is easy and on the basis of previous material balance degree of separation is assumed to be 99.9%.

Average Relative Volatility Calculations:

Calculating relative volatility at the top, $T = 64^{\circ}C$

From Antoine equation:

$$\log P_v' = A - \frac{B}{C+T}$$

For methanol

$$\log P_A = 8.08097 - \frac{1582.27}{239.7+64}$$

$$P_A = 743mmHg$$

For water

$$\log P_B = 8.07131 - \frac{1730.63}{233.42+64}$$

$$P_B = 178.84mmHg$$

Relative volatility at the top:

$$\alpha_{Top} = P_A/P_B$$

$$= 743/178.84$$

$$= 4.15$$

Calculating relative volatility at the bottom, $T = 100^{\circ}C$

From Antoine equation:

$$\log P_v' = A - \frac{B}{C+T}$$

For methanol:

$$\log P_A = 8.08097 - \frac{1582.27}{239.7+100}$$

$$P_A = 2648.72 \text{ mmHg}$$

For water:

$$\log P_B = 8.07131 - \frac{1730.63}{233.42+100}$$

$$P_B = 759.92 \text{ mmHg}$$

Relative volatility at the Bottom:

$$\alpha_{Bottom} = P_A/P_B$$

$$= 2648.72/759.92$$

$$= 3.48$$

$$\alpha_{avg} = \sqrt{\alpha_{top} \times \alpha_{bottom}}$$

$$, \quad = \sqrt{4.15 \times 3.48}$$

$$= 3.8$$

Average relative volatility, $\alpha_{avg} = 3.8$

7.3.1 Determination of minimum Reflux ratio:

Boiling point at 1 bar:

Normal boiling point of methanol = $64.7^{\circ}C$

Normal boiling point of water = $100^{\circ}C$

$$t_b = \sum x_i t_{b_i}$$

$$= 0.925 \times 64.7 + 0.075 \times 100$$

$$= 67.35^{\circ}C$$

For Antoine Equation,

$$\log P_v' = A - \frac{B}{C+T}$$

For Methanol, A = 8.08097, B = 1582.27, C = 239.7

For Water, A = 8.07131, B = 1730.63, C = 233.426

First iteration:

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7+67.38}$$

$$P_v' = 846.90 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426+67.35}$$

$$P_w = 207.69 \text{ mmHg}$$

$$\begin{aligned} \sum x_i P_{v_i} &= x_{\text{methanol}} P_v' + x_{\text{water}} P_w \\ &= 0.925 \times 846.9 + 0.075 \times 207.69 \\ &= 798.95 \text{ mmHg} \end{aligned}$$

Since $798.95 > 760$ mm Hg, we go for second iteration:

$$t_b = 64.7^\circ\text{C}$$

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7+64.7}$$

$$P_v' = 763.78 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426+64.7}$$

$$P_w = 184.62 \text{ mmHg}$$

$$\begin{aligned} \sum x_i P_{v_i} &= x_{\text{methanol}} P_v' + x_{\text{water}} P_w \\ &= 0.925 \times 763.78 + 0.075 \times 184.62 \end{aligned}$$

$$= 720.34 \text{ mmHg}$$

Since $720.34 < 760$ mm Hg, we go for third iteration:

$$t_b = 65.8^\circ\text{C}$$

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7 + 65.8}$$

$$P_v' = 797.42 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426 + 65.8}$$

$$P_w = 193.91 \text{ mmHg}$$

$$\begin{aligned} \sum x_i P_{v_i} &= x_{\text{methanol}} P_v' + x_{\text{water}} P_w \\ &= 0.925 \times 797.42 + 0.075 \times 193.91 \\ &= 752.1 \text{ mmHg} \end{aligned}$$

Since $752.1 < 760$ mm Hg, we go for fourth iteration:

$$t_b = 66.4^\circ\text{C}$$

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7 + 66.4}$$

$$P_v' = 816.28 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426 + 66.4}$$

$$P_w = 199.15 \text{ mmHg}$$

$$\begin{aligned} \sum x_i P_{v_i} &= x_{\text{methanol}} P_v' + x_{\text{water}} P_w \\ &= 0.925 \times 816.25 + 0.075 \times 199.15 \\ &= 769.95 \text{ mmHg} \end{aligned}$$

Since $769.95 > 760$ mm Hg, we go for fifth iteration:

$$t_b = 66.1^\circ C$$

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7+66.1}$$

$$P_v' = 806.8 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426+66.1}$$

$$P_w = 196.46 \text{ mmHg}$$

$$\sum x_i P_{v_i} = x_{\text{methanol}} P_v' + x_{\text{water}} P_w$$

$$= 0.925 \times 806.8 + 0.075 \times 196.46$$

$$= 761.02 \text{ mmHg}$$

Since $761.02 > 760$ mm Hg, we go for sixth iteration:

$$t_b = 66.08^\circ C$$

$$\log P_v' = 8.08097 - \frac{1582.27}{239.7+66.08}$$

$$P_v' = 806.18 \text{ mmHg}$$

$$\log P_w = 8.07131 - \frac{1730.63}{233.426+66.08}$$

$$P_w = 196.34 \text{ mmHg}$$

$$\sum x_i P_{v_i} = x_{\text{methanol}} P_v' + x_{\text{water}} P_w$$

$$= 0.925 \times 806.18 + 0.075 \times 196.34$$

$$= 760.44 \text{ mmHg}$$

Therefore, Final Value is ($t_b = 66.08^\circ C$)

$$\begin{aligned} \text{Average temperature} &= (66.08 + 38)/2 \\ &= 52.04^\circ\text{C} = 325.04^\circ\text{K} \end{aligned}$$

Specific heat capacity at $T = 325.04^\circ\text{K}$

• Methanol

$$C_p^m = C_1 + C_2T + C_3T^2 + C_4T^3$$

$$\begin{aligned} C_p^m &= 105800 - 362T + 0.9379T^2 \\ &= 87225.59\text{J/KmolK} \\ &= 87.22559\text{KJ/KmolK} \end{aligned}$$

• Water

$$\begin{aligned} C_p^w &= C_1 + C_2T + C_3T^2 + C_4T^3 + C_5T^4 \\ C_p^w &= 2.7637 - 2090.1T + 8.125T^2 - 0.014116T^3 + 0.00000937T^4 \\ &= 410294.02\text{J/KmolK} \\ &= 410.29\text{KJ/KmolK} \end{aligned}$$

$$\text{Latent Heat} = \Delta H_r = C_1 \times (1 - T_r)^{C_2 + C_3 \times T_r + C_4 \times T_r^2}$$

• Methanol

$$T_r = T/T_c$$

$$T = 339.08^\circ\text{K}$$

$$T_c = 512.64^\circ\text{K}$$

$$T_r = 0.661$$

$$\Delta H_r = 5.239 \times 10^{-7} \times (1 - 0.661)^{0.35632}$$

$$= 3567.015 \text{ KJ/Kmol}$$

• Water

$$T_r = T/T_c$$

$$T = 339.08^\circ \text{K}$$

$$T_c = 647.13^\circ \text{K}$$

$$T_r = 0.523$$

$$\Delta H_r = 5.205 \times 10^7 \times (1 - 0.523)^{0.3799 - (0.212)(0.523) + (0.2579)(0.523)^2}$$

$$= 40483.79 \text{ KJ/Kmol}$$

Component	C_P Value at 325.04°K , KJ/Kmol K	Latent Heat at 339.08°K , KJ/Kmol K
Methanol	87.225	3567.015
Water	410.29	40483.79

TABLE 7.3: Distillation Column components Heat

Average molar heat capacity:

$$C_p^{avg} = (0.925)(87.225) + (0.075)(410.29)$$

$$= 111.45 \text{ KJ/Kmol K}$$

Average latent heat:

$$\lambda^{avg} = (0.925)(3567.015) + (0.075)(40483.79)$$

$$= 6335.77 \text{ KJ/Kmol}$$

$$q = \frac{H_G - H_F}{H_G - H_L}$$

$$= \frac{\lambda^{avg} + C_p^{avg} \Delta T}{\lambda^{avg}}$$

$$= \frac{6335.77 + (111.45)(66.08 - 38)}{6335.77}$$

$$= 1.49$$

$$\frac{R_M Z_F + q x_D}{R_M(1 - Z_F) + q(1 - x_D)} = \frac{\alpha_{avg} [x_D(q - 1) + Z_F(R_M + 1)]}{(1 - x_D)(q - 1) + (1 - Z_F)(R_M + 1)}$$

$$Z_F = 0.925$$

$$x_D = 0.999$$

$$\alpha_{avg} = 3.8$$

$$q = 1.49$$

$$\frac{R_M(0.925)+(1.49 \times 0.999)}{R_M(0.075)+(1.49 \times 0.001)} = \frac{3.8[(0.999 \times 0.49)+(0.925 \times (R_M+1))]}{(R_M+1)0.075+(0.49 \times 0.001)}$$

$$0.263625R_M^2 + 0.40798135R_M + 0.0080073 = 0.069375R_M^2 + 0.18143R_M + 0.112344$$

$$0.19425R_M^2 + 0.22655R_M - 0.1043 = 0$$

$$R_M = 0.353$$

Minimum reflux ratio, $R_M = 0.353$

7.3.2 Determination of Optimum Reflux Ratio

Optimum Reflux Ratio, $R = 1.5 \times R_M$

$$= 0.53$$

7.3.3 Calculation of number of trays

Methanol in top product, $x_D = 0.999$

Methanol in bottom product, $x_W = 0.012$

Average relative volatility, $\alpha_{avg} = 3.8$

Applying Fenske equation,

$$N_m + 1 = \frac{\log \frac{x_D(1-x_W)}{x_W(1-x_D)}}{\log \alpha_{avg}}$$

$$= \frac{\log \frac{0.999(1-0.012)}{0.012(1-0.999)}}{\log 3.8}$$

$$N_m = 7.64$$

Hence, minimum number of trays required are = 8

Now, minimum reflux ratio, $R_m = 0.353$

And reflux ratio, $R = 0.53$

$$\psi = \frac{R-R_m}{R+1}$$

$$= \frac{0.53-0.353}{0.53+1}$$

$$= 0.115$$

Now, calculating actual number of ideal trays

$$\begin{aligned} f(N) &= \frac{N-N_m}{N+1} = 1 - \exp \left[\left\{ \frac{(1+54.4\psi)}{11+117.2\psi} \right\} \left\{ \frac{\psi-1}{\psi^{0.5}} \right\} \right] \\ &= \frac{N-8}{N+1} = 1 - \exp \left[\left\{ \frac{(1+54.4 \times 0.115)}{11+117.2 \times 0.115} \right\} \left\{ \frac{0.115-1}{0.115^{0.5}} \right\} \right] \\ &= 18.5 \approx 19 \end{aligned}$$

Ideal number of trays = 19

Chapter 8

Process Design of Distillation Column

$$\begin{aligned}\text{Average molar mass of feed} &= 0.925 \times 32 + 0.075 \times 18 \\ &= 30.95 \text{ Kg/Kmol}\end{aligned}$$

Feed to the column:

$$CH_3OH = 521.35 \text{ Kmol/hr}$$

$$H_2O = 41.74 \text{ Kmol/hr}$$

$$F = 563.09 \text{ Kmol/hr}$$

$$D = 520.87 \text{ Kmol/hr}$$

$$W = 42.22 \text{ Kmol/hr}$$

$$R = 0.53 \text{ Kmol/hr}$$

$$q = 1.49 \text{ Kmol/hr}$$

Molar flow rates of vapor and liquid at the top (enriching section)

$$L = R.D = 0.53 \times 520.87 = 276.06 \text{ Kmol/hr}$$

$$V = (R + 1).D = 1.53 \times 520.87 = 796.93 \text{ Kmol/hr}$$

Molar flow rates of liquid and vapor at the bottom (stripping section)

$$\bar{L} = L + F.q = 276.06 + 563.09 \times 1.49 = 1109.06 \text{ Kmol/hr}$$

$$\bar{V} = F(q - 1) + V = 563.09(1.49 - 1) + 796.93 = 1072.84 \text{ Kmol/hr}$$

8.1 Column Diameter

8.1.1 Top Diameter of the Column

Operating pressure at the Top = 1 bar = 101.325 KPa

Since it is a total condenser, Reflux = output of column

$$\frac{L_W}{V_W} = \frac{L}{V} = \frac{270.06}{796.93} = 0.338$$

L_W and V_W are Mass flow rates of liquid and vapour at the top

- Density of the vapor, ρ_V

$$\rho_V = \frac{\phi M_{av}}{RT}$$

$$M_{av} = \sum x_i M_i$$

$$x_1 = \frac{520.83}{520.87} = 0.999$$

$$x_2 = \frac{0.042}{520.87} = 8.063 \times 10^{-5}$$

$$M_{av} = (0.999)(32) + (8.063 \times 10^{-5})(18)$$

$$M_{av} = 33.44 \text{ Kg/Kmol}$$

$$\rho_V = \frac{33.44}{64+273} \times \frac{273}{22.414}$$

$$\rho_v = 1.21 \text{ Kg/m}^3$$

- Density of liquid, ρ_L

$$\rho_L = \frac{1}{\sum \frac{w_i}{\rho_i}}$$

$$\text{Density of pure water } 64^\circ\text{C} = 981.09 \text{ Kg/m}^3$$

$$\text{Density of pure methanol } 64^\circ\text{C} = 751.4 \text{ Kg/m}^3$$

$$\text{Density of pure methanol } 50^\circ\text{C} = 764.8 \text{ Kg/m}^3$$

$$\text{Density of pure methanol } 70^\circ\text{C} = 746.2 \text{ Kg/m}^3$$

$$= 751.4 \text{ Kg}/m^3$$

$$\text{Total Moles} = 520.83 + 0.042$$

$$= 520.872 \text{ Kmol}$$

$$\text{Total weight of } CH_3OH = (520830)(32)(0.001) \text{ Kg}$$

$$= 16666.56 \text{ Kg}$$

$$\text{Total weight of water} = 0.042 \times 18$$

$$= 0.756 \text{ Kg}$$

$$W_M = \frac{16666.56}{16666.56 + 0.756} = 0.999$$

$$W_W = 0.001$$

$$\rho_L = \frac{1}{\frac{0.999}{751.4} + \frac{0.001}{981.09}} = 751.57 \text{ Kg}/m^3$$

- Liquid vapor flow factor at top

$$F_{LV} = \frac{L_W}{V_W} \left(\frac{\rho_V}{\rho_L} \right)^{0.5}$$

$$= 0.338 \left(\frac{1.21}{751.57} \right)^{0.5}$$

$$= 0.0135$$

Considering tray spacing = 0.3 m

$$C_f = 0.055 \text{ (from Graph)}$$

$$V_f = C_f \left(\frac{\sigma}{0.02} \right)^{0.2} \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5}$$

- Calculation of " σ_{Me} "

Parachor values of Methanol :

$$(-CH_3) \text{ Contribution} = 55.5$$

$$(-OH) \text{ Contribution} = 29.0$$

$$[P] = 85.3$$

$$\sigma_W = 58 \times 10^{-3} \text{ N}/m$$

$$\sigma_{CH_3OH}^{0.25} = [P] (\rho'_L - \rho'_V)$$

$$\rho'_L = \frac{\text{Density of pure liquid methanol}}{\text{Molecular wt.}}$$

$$\rho'_V = \frac{1}{273+64} \times \frac{273}{22414} = 3.61 \times 10^{-5} \text{ mol}/cm^3$$

$$\sigma_{Meth}^{0.25} = (85.3)(0.0234 - 0.0000361)$$

$$\sigma_{Meth} = 15.74 \text{ dyne/cm}$$

$$\sigma_{Meth} = 0.01574 \text{ N/m}$$

$$\sigma = \sum x_i \sigma_i$$

$$= (0.999)(0.01574) + (8.063 \times 10^{-5})(0.058) = 15.734 \times 10^{-3}$$

- Calculation of flooding velocity, V_F

$$V_F = C_f \left(\frac{a}{0.02} \right)^{0.5} \left(\frac{\rho_L - \rho_V}{\rho_V} \right)$$

$$= (0.055) \left(\frac{15.734}{0.02} \right)^{0.2} \left(\frac{751.57 - 1.21}{1.21} \right)^{0.5}$$

$$= 1.305 \text{ m/sec}$$

$$\text{Let velocity at top} = 0.85 V_F$$

$$= 1.109 \text{ m/sec}$$

- Volumetric flow rate at top

$$\varphi = \frac{V M_{av}}{\rho_{av}}$$

$$= \frac{(796.93)(33.44)}{1.21}$$

$$= 6.117 \text{ m}^3/\text{sec}$$

- Net area required at the top

$$A_n = \frac{\varphi}{V} = \frac{6.117}{1.305} = 4.687 \text{ m}^2$$

- Let downcomer area

$$A_d = 0.12 A_c$$

$$A_n = A_c - A_d$$

$$= 0.88 A_c$$

$$\text{Therefore } A_c = \frac{4.687}{0.88}$$

$$A_c = 5.326 \text{ m}^2$$

$$\text{Inside diameter of column} = \sqrt{\frac{4 A_c}{\pi}}$$

$$i_d = 2.6 \text{ m}$$

8.1.2 Bottom diameter of the Column

$$\Delta p_t = 0.4 \text{ bar [for sieve trays]}$$

$$\text{Bottom pressure} = \Delta p_t + \text{operating pressure at the top}$$

$$= 1.4 \text{ bar}$$

$$\text{Calculated base temperature, } t_b = 108.5^\circ \text{C}$$

Molar flow rates of liquid and vapor at bottom

$$\bar{L} = 1109.06 \text{ kmol/hr}$$

$$\bar{V} = 1072.84 \text{ kmol/hr}$$

$$\frac{\bar{L}}{\bar{V}} = \frac{1109.06}{1072.84} = 1.03$$

• *Density of Vapor' ρ_V' at bottom*

$$\rho_V = \frac{pM_{av}}{RT}$$

$$M_{av} = \sum x_i M_i$$

Bottom

$$x_1 = 0.0123$$

$$x_2 = 0.987$$

$$M_{av} = (0.0123)(32) + (0.987)(18)$$

$$= 18.159$$

$$\rho_V = \frac{140 \times 18.159}{273 + 108.5} \times \frac{273}{101.325 \times 22.414}$$

$$\rho_V = 0.801 \text{ Kg/m}^3$$

• *Density of liquid at bottom*

$$\rho_L = \frac{1}{\sum \frac{w_i}{\rho_i}}$$

At 1.4 bar

$$\text{Density of water } 108.5 = 951.25 \text{ Kg/m}^3$$

$$\text{Density of methanol } 108.5 = 705.65 \text{ Kg/m}^3$$

$$W_{MeOH} = \frac{16.64}{750.6 + 16.64} = 0.021$$

$$W_{H_2O} = \frac{750.6}{750.6 + 16.64} = 0.978$$

$$\rho_L = \frac{1}{\frac{0.021}{705.65} + \frac{0.978}{951.25}} = 945.28 \text{ Kg/m}^3$$

• *Liquid Vapor flow factor at bottom $[F_{LV}]$*

$$F_{LV} = \frac{\bar{L}}{\bar{V}} \left(\frac{\rho_V}{\rho_L} \right)^{0.5}$$

$$= 1.03 \times \left(\frac{0.801}{945.28} \right)^{0.5}$$

$$= 0.03$$

• *Calculation of flooding velocity' V_f'*

For tray spacing = 0.3 m

from graph; $C_f = 0.051$

$$\sigma_{meth} = 0.0147 \text{ N/m}$$

At 108.5°C

$$\sigma_{H_2O} = 0.0573 \text{ N/m}$$

At 108.5°C

$$\sigma = \sum x_i \sigma_i$$

$$= 0.05673 \text{ N/m}$$

$$V_f = C_f \left(\frac{a}{0.02} \right)^{0.2} \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5} = 2.157 \text{ m/sec}$$

$$V_f = 2.157 \text{ m/sec}$$

Let actual flooding vapor velocity = 0.85×2.157

$$= 1.833 \text{ m/sec}$$

Volumetric flow rate at bottom

$$\varphi = \frac{\bar{V} M_{av}}{\rho_V} = \frac{1072.84 \times 18.159}{0.801}$$

$$= 243091.2 \text{ m}^3/\text{hr}$$

$$= 6.75 \text{ m}^3/\text{sec}$$

Net area required at the top :

$$A_n = \frac{\varphi}{V_{f,actual}} = \frac{6.75}{1.833}$$

$$= 3.68 \text{ m}^2$$

$$A_c = \frac{A_n}{0.88} = 4.18 \text{ m}^2$$

$$\text{Inside diameter at bottom} = \sqrt{\frac{4A_c}{\pi}} = 2.31 \text{ m}$$

• Calculation of shell thickness

$$\text{Thickness, } t = \frac{P_i D_i}{2Jf - P_i}$$

MOC:

Semi – killed or silicon killed carbon steel

Top operating conditions

$$P = 1 \text{ bar} \Rightarrow \text{Design pressure} = 0.1P$$

$$P_i = 1.1 \text{ bar}$$

$$f = 133 \text{ N/mm}^2$$

$$D_i = 2.6 \text{ m}$$

for Single weld butt joint with bonding strips and for Degree of Radiography = 0.8

$$J = 0.8$$

$$t = \frac{(0.11)(2600)}{(1.6)(133) - 0.11} = 1.3 \text{ mm}$$

for corrosion allowance of 2 mm

$$t_{top} = 2 + 1.3 = 3.3 \text{ mm}$$

• Bottom Operating Conditions

$$P = 1.4 \text{ bar}$$

$$T = 108.5^\circ\text{C}$$

$$\text{Design Pressure} = 1.1P$$

$$= 1.1 \times 1.4$$

$$= 1.54 \text{ bar} = 0.154 \text{ N/mm}^2$$

$$D_i = 2.3 \text{ m}$$

$$f = 125 \text{ N/mm}^2$$

$$t_{bottom} = \frac{0.154 \times 2310}{2 \times 125 - 0.154}$$

$$= 1.42 \text{ mm}$$

for corrosion allowance = 2 mm

$$t_{bottom} = 1.42 + 2 = 3.42 \text{ mm}$$

• Calculation of height of tower = 0.3 m

for tray spacing = 0.3 m

$$\text{for tray efficiency} = 85 \text{ Actual number of trays} = \frac{19(\text{ideal no. of trays})}{0.85}$$

$$= 22.5 \approx 23$$

$$\text{Height of tower} = 0.3 \times (23 + 1)$$

$$= 7.2 \text{ m}$$

Chapter 9

Cost Estimation of Distillation Column Section

9.1 Introduction

Here, the cost estimation of the distillation tower has been done in which the Total Capital Investment has been estimated using various cost correlation formulas.

The Equipments whose costs are to be calculated are:

1. Distillation column shell
2. Tower Internals
3. Condenser
4. Reboiler

The Correlations used here are Guthrie's Cost Correlations.

9.2 Cost Calculations

Using Guthrie's Correlations for:

9.2.1 Distillation column shell

$$\begin{aligned}\text{Column Shell Cost} &= \left(\frac{M\&S}{280}\right) [101.9D^{1.066}H^{0.82}F_C] \\ &= \left(\frac{1387.8}{280}\right) [101.9 \times (2.543 \times 3.2)^{1.066} \times (7 \times 3.2)^{0.82} \times 1.0] \\ &= 58,137.16 \$\end{aligned}$$

= Rs. 36,20,201.46 Where, $F_C = F_M F_P$ are the correction factors for MOC and Pressure respectively

M&S: Marshall and Swift Index

D: Diameter of the column, in ft

H: Height of the column, in ft

9.2.2 Tower Internals

$$\begin{aligned}\text{Tower Internals Cost} &= \left(\frac{M\&S}{280}\right) [4.7D^{1.55}HF_C] \\ &= \left(\frac{1387.8}{280}\right) [4.7 \times (2.543 \times 3.2)^{1.55} (7 \times 3.2) \times 2.2]\end{aligned}$$

Where, $F_C = F_S + F_T + F_M$

$$F_S(\text{tray spacing}) = 2.2$$

$$F_T(\text{tray type}) = 0.0$$

$$F_M(\text{tray material}) = 0.0$$

H : Height of tray stack

$$\text{Total cost} = \text{Rs.} 45,14,906.25$$

Now, Assuming 20% delivery cost of the column

$$\text{Total delivered equipment cost} = \text{Rs.} 54,17,887.5$$

9.2.3 Condenser

Column outlet flow rate = 796.83 Kmol/hr

$$\text{Area}(\text{approx.}) = 482.36m^2$$

$$= 4939.36ft^2$$

$$\text{Condenser Cost} = \left(\frac{M\&S}{280}\right) [101.3A^{0.65}F_C]$$

$$= \left(\frac{1387.8}{280}\right) [101.3(4939.6)^{0.65} \times 0.8]$$

$$= \text{Rs.} 62,95,546$$

Where, $F_C = (F_D + F_P)F_M$

Assuming a Fixed tube Heat exchanger

$$F_D(\text{design type}) = 0.8$$

$$F_P = 0.0$$

$$F_M = 1.0$$

Total cost including delivery charges = Rs.75, 54, 656

9.2.4 Reboiler

$$\text{Area}(\text{approx.}) = 1684.19 \text{ ft}^2$$

$$\text{Reboiler Cost} = \left(\frac{M\&S}{280}\right) [101.3A^{0.65}F_C]$$

$$= \left(\frac{1387.8}{280}\right) [101.3 \times 1684.19^{0.65}0.8]$$

$$= \text{Rs.}31, 28, 253$$

$$\text{Delivered Cost} = \text{Rs.}37, 53, 903$$

Thus, the total purchased equipment delivered cost(E)

=distillation column cost + Reboiler cost + Condenser cost

$$= \text{Rs.}1,67,26,446$$

Purchased equipment installation cost, $39\%E = \text{Rs.}1.672 \times 10^7$

Instrumentation, $28\%E = \text{Rs.}0.46816 \times 10^7$

Electrical installation, $10\%E = \text{Rs.}0.1672 \times 10^7$

Piping installation, $31\%E = \text{Rs.}0.51832 \times 10^7$

Buildings including services, $22\%E = \text{Rs.}0.36784 \times 10^7$

Service facilities, $55\%E = \text{Rs.}0.9196 \times 10^7$

Land, $6\%E = 0.10032 \times 10^7$

Thus, total cost, D = $\text{Rs.}4.86344 \times 10^7$

Engineering & supervision, $32\%E = \text{Rs.}0.53504 \times 10^7$

Construction Expenses, $34\%E = \text{Rs.}0.56848 \times 10^7$

Total indirect investment, I = $\text{Rs.}1.10352 \times 10^7$

Thus, D + I = $\text{Rs.}5.96696 \times 10^7$

Contractors fee, $5\%(D + I) = \text{Rs.}0.29034 \times 10^7$

Contingency, $10\%(D + I) = Rs.0.596696 \times 10^7$

Therefore, FCI = $Rs.6.86 \times 10^7$

Working Capital Cost, $15\%TCI = Rs.1.2109 \times 10^7$

Total Capital Investment = Rs.8,07,29,000

Chapter 10

Results and Discussion

Mass balance results:

Final output = 400 tonnes/day (520 Kmol methanol/day)

Percentage Purity = 98.9%

Product composition:

Top:

$CH_3OH = 520.83$ Kmol/hr

$H_2O = 0.042$ Kmol/hr

Bottoms:

$CH_3OH = 0.52$ Kmol/hr

$H_2O = 41.7$ Kmol/hr

Distillation column

Amount of product stream = 526.62 Kmol/hr

Inlet feed flow rate = 639.312 Kmol/hr

Reactor

Percentage overall conversion in reactor = 59.5% ($CO_2 + CO$ basis)

Total feed to the reactor = 3280.37 Kmol/hr

Reactor output :

$CH_3OH = 521.35$ Kmol/hr

$H_2O = 41.76$ Kmol/hr

$CO = 271.61$ Kmol/hr

$$CO_2 = 187.86 \text{ Kmol/hr}$$

$$H_2 = 1133.06 \text{ Kmol/hr}$$

$$CH_4 = 72.17 \text{ Kmol/hr}$$

$$N_2 = 9.841 \text{ Kmol/hr}$$

Feed composition:

$$\text{Feed Flow Rate required} = 1683.34 \text{ Kmol/hr}$$

Heat Balance Results: Feed Stream:

$$\text{Energy of feed stream } (T_{ref} = 25^\circ C) = 1227130.657 \text{ kcal/hr}$$

Compressor:

$$\text{Value of } \gamma = 1.43$$

After Mixing:

$$\text{Energy of the stream after mixing with recycle stream} = 1380657.174 \text{ kcal/hr}$$

Also, this is the energy that stream carries before entering into FEHE.

$$\text{The Temperature of the stream} = 83^\circ C$$

Reactor:

$$\text{Energy of the inlet stream} = 5243784.244 \text{ kcal/h}$$

$$\text{Temperature of the inlet stream} = 241^\circ C$$

$$\text{Energy of the exit stream} = 7698557.586 \text{ kcal/hr}$$

$$\text{Temperature of the exit stream} = 267^\circ C$$

Distillation column Results:**Pressure**

$$\text{Operating Pressure} = 1 \text{ bar}$$

$$\text{Overall Pressure drop} = 0.4 \text{ bar}$$

Temperature

Top Temperature = $64^{\circ}C$

Bottom Temperature = $108.5^{\circ}C$

Degree of separation: 99.9%

Average relative volatility $\alpha_{avg} = 3.8$

Optimum Reflux Ratio = 0.53

Ideal number of trays = 19

Inside diameter at the top = 2.6 m

Inside diameter at the bottom = 2.31 m

Height of tower = 7.31 m

Economic Estimations

Fixed Capital Investment required = Rs. 6,86,00,000/-

Working Capital Investment required = Rs. 1,21,29,000/-

Thus, **Total Capital Investment required = Rs. 8,07,29,000/-**

Chapter 11

Conclusion

The designing of the Process Flow Diagram of the plant for producing methanol along with the material and energy balance across all the equipment, selection of the type of process and the reactor was successfully done.

Also, the entire distillation column plant was designed and the cost estimation was successfully done and reported.

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