# **PRODUCTION OF ETHYLENE OXIDE**

Submitted in the partial fulfilment of

The requirements for the degree of

# **BACHELOR OF TECHNOLOGY**

in CHEMICAL ENGINEERING

of
ASSAM SCIENCE AND TECHNOLOGY UNIVERSITY



# SUBMITTED BY

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DEPARTMENT OF CHEMICAL ENGINEERING

ASSAM ENGINEERING COLLEGE

JALUKBARI, GUWAHATI – 781013

**JUNE 2022** 

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# <u>CERTIFICATE</u> DEPARTMENT OF CHEMICAL ENGINEERING

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Dr. Kabita Chakrabarty

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Ms. Mousumee Das

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### **ACKNOWLEDGEMENT**

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- Pinakshi Kalita (18105)
- Darsana Saud (18260)
- Ananya Saikia (18275)
- Prastuti Devi (18362)

### **ABSTRACT**

Ethylene oxide, the target product of the present work is a flammable, colourless gas or liquid with the molecular formula C<sub>2</sub>H<sub>4</sub>O. Ethylene oxide is found in the production of solvents, antifreeze, textiles, detergents, adhesives, polyurethane foam, and pharmaceuticals. The present work illustrates the production of Ethylene oxide by different production methods, literature survey and selection of an appropriate method. The method of production we have chosen is oxygen based direct oxidation process. The mass balance and energy balance are being performed for the various units involved in the production of ethylene oxide. In design section we have designed a pressure vessel and heat exchanger which matches the design specifications required for given plant.

# **PROJECT AT A GLANCE**

# Title: Production of Ethylene Oxide

### PLANT CAPACITY

### 1. PRODUCT

a) Plant capacity	10,000 ton/annum
b) Work days in a year	330 days
c) Production rate of ethylene per hour	1262.626 kg/hr
2. FRESH FEED	2749.201 kg/hr
	= 86.956 kmol/hr
Constituents	
$C_2H_4$	114.7 kg/hr
O <sub>2</sub>	1308.47 kg/hr
Inerts	25.70 kg/hr
3. DESIGN ASPECTS	
a) 1-2 shell and tube Heat exchanger	
Shell side	
ID of shell used	$2 \ 1\frac{1}{4}$ in
Baffle spacing	5
Shell pass	1
Pressure drop	4.5 psi
Tube side	
Number of tubes	160

### Tube specification

OD, Pitch, BWG	$\frac{3}{4}$ , OD, 1" sq pitch, 16 BWG
No. of passes	2
Overall heat transfer co-efficient	37.36 Btu/hr ft <sup>2</sup> °F
Dirt factor	0.0001
Pressure drop	4.439 psi
b) Pressure vessel	
Standard plate thickness for spherical sh	nell 5 mm
Thickness of a compensated standard di	shed head 12 mm
Type of weld	double welded butt joint

# 4. EQUIPMENT USED

Reactor, EO absorber, CO<sub>2</sub> absorber, CO<sub>2</sub> stripper, 1-2 shell and tube Heat Exchanger, Distillation Column, Pressure Vessel, Compressor

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#### CHAPTER 1

# **INTRODUCTION**

Ethylene oxide is an important raw material for making major consumer goods in virtually all industrialized countries. Ethylene oxide (oxirane) is the simplest cyclic ether. Ethylene oxide (EO) is one of the epoxide family of chemicals. Ethylene oxide is very reactive because its highly strained ring can be opened easily, and is thus one of the most versatile chemical intermediates. Because of its reactivity and toxicity, it is also a hazardous compound that has been involved in a number of serious incidents.

Ethylene oxide was prepared by eliminating hydrochloric acid from ethylene chlorohydrin, using potassium hydroxide solution. Industrial production by the chlorohydrin process began in 1914. The Ethylene Chlorohydrin process involves the reaction of ethylene with hypochlorous acid followed by dehydrochlorination of the resulting chlorohydrin with lime to produce ethylene oxide and calcium chloride. The chlorohydrin process is not economically competitive, and was quickly replaced by the direct oxidation process as the dominant technology. At the present time, all the ethylene oxide production in the world is achieved by the direct oxidation process. The direct oxidation technology, utilizes the catalytic oxidation of ethylene with oxygen over a silver-based catalyst to yield ethylene oxide. The process can be divided into two categories depending on the source of the oxidizing agent: the air-based process and the oxygen-based process. In the first, air or air enriched with oxygen is fed directly to the system. In the second, a high purity oxygen stream (>95 mol %) from an air separation unit is employed as the source of the oxidizing agent. Currently about 98% of world ethylene oxide capacity is based on the direct oxidation route.

#### **1.1. OCCURRENCE**

#### **1.1.1. Natural occurrence**

Ethylene oxide occurs endogenously as a metabolite of ethylene in certain plants and micro-organisms. Ethylene oxide can be generated from water-logged soil, manure and sewage sludge, but emissions are expected to be negligible.

#### **1.1.2. Occupational exposure**

Occupational exposures are related to the production of ethylene oxide and its use in chemical and allied products industry (manufacture of plastics, synthetic materials and drugs) and hospital sterilization.

#### **1.2. RAW MATERIAL SOURCES OF ETHYLENE OXIDE**

#### 1.2.1. Ethylene

Ethylene is produced from the cracking of fractions obtained from distillation of natural gas and petroleum; it is a naturally occurring hormone in plants, in which it inhibits growth and promotes leaf fall and in fruits, it promotes ripening.

#### 1.2.2. Oxygen

Air contains 21% of oxygen and the principle source of oxygen in industry is fractional distillation of liquid air. There are several other commercial methods for oxygen production in industries.

#### **1.3. STRUCTURE**

Ethylene oxide is an organic compound with the formula C2H4O. It is a cyclic ether and the simplest epoxide: a three-membered ring consisting of one oxygen atom and two carbon atoms.

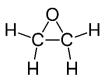


Figure 1.1:

### **1.4. PHYSICAL PROPERTIES**

Ethylene oxide is an organic compound with the formula  $C_2H_4O$ . Ethylene oxide is a colourless and flammable gas or liquid with a faintly sweet odour. Ethylene oxide is a colourless gas at 25 °C (77 °F) and is a mobile liquid at 0 °C (32 °F). Viscosity of liquid ethylene oxide at 0 °C is about 5.5 times lower than that of water. Boiling point of this compound is 10.4°C and melting point is -112.5°C. The Density at 25°C is 0.882 g/mL Ethylene oxide is readily soluble in water, ethanol, diethyl ether and many organic solvents.

Table 1.1:

Property	Value
Molecular weight	44.05 g/mol
Physical state (room temperature)	Gaseous
Melting Point	-112.44°C
Boiling Point	10.5°C

Density	882 kg/m <sup>3</sup>
Viscosity, (centipoises at 4°C)	0.31
Specific heat (Cal/°C-g at 20°C)	0.44
Solubility	Completely soluble in water, acetone,
	benzene, carbon tetrachloride, ether,
	methanol.
Reactivity	Potentially explosive when heated or when in
	the presence of alkali metal hydroxides and
	highly active catalytic surfaces.

### **1.5. CHEMICAL PROPERTIES**

#### 1.5.1. Addition of water and alcohols

Aqueous solutions of ethylene oxide are rather stable and can exist for a long time without any noticeable chemical reaction, but adding a small amount of acid, such as strongly diluted sulfuric acid, immediately leads to the formation of ethylene glycol, even at room temperature:

 $(CH_2CH_2) O + H_2O \rightarrow HO - CH_2CH_2 - OH$ 

The reaction also occurs in the gas phase, in the presence of a phosphoric acid salt as a catalyst.

Reactions of ethylene oxide with fatty alcohols proceed in the presence of sodium metal, sodium hydroxide or boron trifluoride and are used for the synthesis of surfactants

#### 1.5.2. Addition of carboxylic acids and their derivatives

Reactions of ethylene oxide with carboxylic acids in the presence of a catalyst results in glycol mono- and diesters:

 $(CH_2CH_2) O + CH_3CO_2H \rightarrow HOCH_2CH_2 - O_2CCH_3$ 

 $(CH_2CH_2) O + (CH_3CO)_2O \rightarrow CH_3CO_2CH_2CH_2O_2CCH_3$ 

The addition of acid amides proceeds similarly:

 $(CH_2CH_2) O + CH_3CONH_2 \rightarrow HOCH_2CH_2NHC(O)CH_3$ 

#### 1.5.3. Adding ammonia and amines

Ethylene oxide reacts with ammonia forming a mixture of mono-, di- and triethanolamines. The reaction is stimulated by adding a small amount of water.

 $(CH_2CH_2) O + NH_3 \rightarrow HO-CH_2CH_2-NH_2$ 

 $2 (CH_2CH_2) O + NH_3 \rightarrow (HO-CH_2CH_2)_2NH$ 

 $3 (CH_2CH_2) O + NH_3 \rightarrow (HO-CH_2CH_2)_3N$ 

#### 1.5.4. Halide addition

Ethylene oxide readily reacts with aqueous solutions of hydrochloric, hydrobromic and hydroiodic acids to form halohydrins. The reaction occurs easier with the last two acids:

 $(CH_2CH_2) O + HCl \rightarrow HO-CH_2CH_2-Cl$ 

#### 1.5.5. Addition of nitrous and nitric acids

Reaction of ethylene oxide with aqueous solutions of barium nitrite, calcium nitrite, magnesium nitrite, zinc nitrite or sodium nitrite leads to the formation of 2-nitroethanol:

$$(\mathrm{CH}_{2}\mathrm{CH}_{2})\mathrm{O} + \overset{\mathrm{nitric}}{\mathrm{HNO}_{3}} \longrightarrow \mathrm{HO} - \mathrm{CH}_{2}\mathrm{CH}_{2} - \mathrm{ONO}_{2} \xrightarrow[-\mathrm{H}_{2}\mathrm{O}]{} \mathrm{O}_{2}\mathrm{NO} - \mathrm{CH}_{2}\mathrm{CH}_{2} - \mathrm{ONO}_{2}$$

2 (CH<sub>2</sub>CH<sub>2</sub>) O + Ca (NO<sub>2</sub>)<sub>2</sub> + 2 H<sub>2</sub>O  $\rightarrow$  2 HO–CH<sub>2</sub>CH<sub>2</sub>–NO<sub>2</sub> + Ca (OH)<sub>2</sub>

#### 1.5.6. Alkylation of aromatic compounds

Ethylene oxide enters into the Friedel–Crafts reaction with benzene to form phenethyl alcohol:



#### 1.5.7. Thermal decomposition

Ethylene oxide is relatively stable to heating – in the absence of a catalyst, it does not dissociate up to 300 °C (572 °F), and only above 570 °C (1,058 °F) there is a major exothermic decomposition, which proceeds through the radical mechanism.<sup>[47]</sup> The first stage involves isomerization, however high temperature accelerates the radical processes. They result in a gas mixture containing acetaldehyde, ethane, ethyl, methane, hydrogen, carbon dioxide, ketene and formaldehyde.<sup>[53]</sup> High-temperature pyrolysis ((830–1,200) K (557–927) °C; (1,034–1,700) °F) at elevated pressure in an inert

atmosphere led to a more complex composition of the gas mixture, which also contains acetylene and propane.

#### **1.6. USES**

Ethylene oxide can be used for various purposes:

- The major use of ethylene oxide is as a chemical intermediate in the manufacture of ethylene glycol.
- It is also used widely in hospitals as a gaseous sterilant for heat-sensitive medical items, surgical instruments and other objects and fluids that come into contact with biological tissues.
- Small amounts of ethylene oxide are used as a fumigant, as a sterilant for food (spices) and cosmetics, and in hospital sterilization of surgical equipment and plastic devices that cannot be sterilized by steam.

#### **1.7. HEALTH IMPACTS**

Ethylene oxide is toxic and a potential human carcinogen. Its vapour is extremely irritating to eyes, causing permanent damage, and to the respiratory tract. Exposure can cause headaches, nausea, damage to lungs and finally coma and death. In contact with skin, blisters are formed and absorption takes place. Sensitization can occur. rubber Non-permeable protective clothing, polychloroprene rubber gloves and boots, chemical goggles and respirators must be worn at all times, and good working practices are essential. PVC and nitrile rubbers have limited resistance to ethylene oxide and should not be used; neither should leather boots which absorb the liquid.

#### **1.8. HAZARDS**

Ethylene oxide is extremely flammable, and its mixtures with air are explosive. When heated it may rapidly expand, causing fire and explosion. Several industrial accidents have been attributed to ethylene oxide explosion.

The autoignition temperature is 429 °C (804 °F), decomposition temperature of 571 °C (1,060 °F) at 101.3 kPa (14.69 psi), minimum inflammable content in the air is 2.7%, and maximum limit is 100%. Ethylene oxide in presence of water can hydrolyse to ethylene glycol and form polyethylene oxide, which then eventually is oxidized by air and leads to hotspots that can trigger explosive decomposition.

Fires caused by ethylene oxide are extinguished with conventional media including foam, carbon dioxide or water. Suppression of this activity can be done by blanketing with an inert gas until total pressure reaches the non-explosive range. Extinguishing of burning ethylene oxide is complicated by its ability to continue burning in an inert atmosphere and in water solutions. Fire suppression is reached only upon dilution with water above 22:1.

#### **1.9. STORAGE AND HANDLING**

Store under an inert gas, such as nitrogen, in a welded stainless-steel container of 4.5 bar minimum working pressure. Storage should be kept well away from the production facilities. Liquid ethylene oxide polymerizes easily in the presence of alkalies, mineral acids, metal chlorides, metal oxides, iron, aluminium or tin. Care is required when transferring ethylene oxide, and all equipment must be free from rust and other contaminants. Regular checks must be made for vapour leakage and build-up prevented by efficient extraction systems. In the event of spills, extinguish all sources of ignition

and evacuate personnel. Contain with dry sand or earth and disperse vapours with a water spray. Ethylene oxide must not be allowed to flow into streams, drains or sewers.

# CHAPTER 2

# **LITERATURE SURVEY**

Ethylene oxide has been produced commercially by two basic routes:

- Ethylene chlorohydrin
- Direct oxidation processes.

The direct oxidation process again is of two types depending on the types of oxidising agent:

- Air based Direct Oxidation Process
- Oxygen based Direct Oxidation Process

### 2.1. ETHYLENE CLOROHYDRIN PROCESS

The process involves the reaction of ethylene with hypochlorous acid followed by dehydrochlorination of the resulting chlorohydrin with lime to produce ethylene oxide and calcium chloride. Chlorohydrin process is comprised of three major steps:

- Synthesis of ethylene chlorohydrin
- Dehydrochlorination of ethylene chlorohydrin to ethylene oxide
- Purification of ethylene oxide

Advantage: Simple process, Higher yield,

**Disadvantages:** most of the chlorine is lost as calcium chloride, which is an unwanted by-product its capital costs are higher, largely due to material of construction

considerations, effluent load high It also causes pollution problems and is not economically competitive.

#### 2.2. DIRECT OXIDATION PROCESS

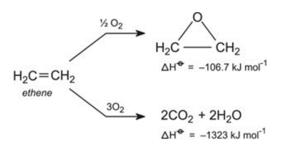
In Direct Oxidation Process, there are no chlorinated hydrocarbon by-products to be sold, processing facilities can be made simpler, and operating costs are lower. Also, there is no need to involve Chlorine for the Production of Ethylene Oxide. The main disadvantage of the direct oxidation process is the lower yield or selectivity of ethylene oxide per unit of feed ethylene consumed. The main inefficiency in the process results from the loss of 20-25% of the ethylene to carbon dioxide and water. Consequently, operating conditions must be carefully controlled to maximize selectivity.

The main reaction is:

$$C_2H_4 + 1/2 O_2 \rightarrow C_2H_4O$$

The only significant by-products are carbon dioxide and water, which are formed either by complete combustion of ethylene:

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



#### 2.2.1. Air Based Direct Oxidation Process

In Air Based Oxidation Process, air or air enriched with oxygen is fed directly to the system. Air introduces a large amount of nitrogen into the recycle gas, which means that a large amount of purge gas must be vented to maintain a constant nitrogen concentration in the recycle stream. The quantity of gas that is vented removes sufficient  $CO_2$  to make  $CO_2$  scrubbing unnecessary. The air-based process has a lower selectivity.

Advantages: It requires lesser amount of pressure than that in oxygen-based process.

**Disadvantages:** Higher initial building cost, Air purification unit required, purge stream required, large reactor required, selectivity is less.

#### 2.2.2. Oxygen Based Direct Oxidation Process

In oxygen based direct oxygen-based process, a high purity oxygen stream (>95 mol %) from an air separation unit is employed as the source of the oxidizing agent. The oxygen-based process uses substantially pure oxygen, reduces the quantities of inert gases introduced into the cycle, and thereby results in almost complete recycle of the unconverted ethylene.

Advantages: Lower capital cost, higher selectivity of catalyst, operation simpler and easier, more economic.

**Disadvantages:** Becomes unattractive if oxygen purity is low.

# CHAPTER 3

# **PROCESS SELECTION AND DESCRIPTION**

### **3.1. PROCESS SELECTION**

This chapter deals with the selection of the process for manufacture of Ethylene Oxide. As per literature survey we have found the following processes. And they are:

- 1) Ethylene Chlorohydrin Process
- 2) Direct Oxidation Process:
- a. In presence of air
- b. In presence of oxygen

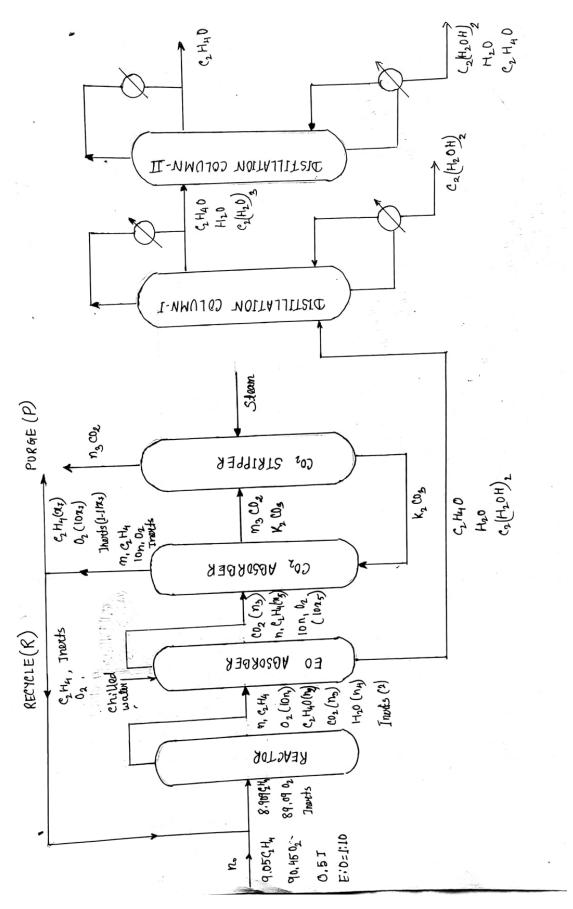
In order to choose a particular process for manufacture of ethylene oxide the following table gives a comparison between the above-mentioned processes based on raw materials, catalyst, temperature, pressure, advantages, disadvantages and yield of the process.

# Table 3.1: COMPARISON OF DIFFERENT PROCESSES

Selection	Chlorohydrin	Air – based Direct	Oxygen – based Direct
criteria		Oxidation	Oxidation
Raw	Ethylene,	Ethylene, air	Ethylene, high purity Oxygen
Materials	hypochlorous acid		
Catalyst	-	Silver based catalyst	Silver based catalyst
Temperature	-	-	200-300°C
Pressure	-	-	10-30 bar
Advantages	Simple process,	-	Lower capital cost,
	yield higher than		Higher selectivity of catalyst,
	oxidation process		Operation is simpler and
			easier,
			More economic.
Disadvantages	Capital costs are	Higher initial	Becomes unattractive if
	higher,	building cost,	oxygen purity is low.
	Chlorine is lost as	Air purification unit	
	unwanted by-	is required,	
	product,	Purge stream	
	Effluent load is	required,	
	high,	Large reactor	
	Not economically	required,	
	active.	Selectivity is less.	
Yield	80%	-	60%

From the above table it is seen that "Direct oxidation process: in presence of oxygen" is the most promising and economic technique for the production of Ethylene Oxide.

# **3.2. FLOWSHEET**



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### **3.3. PROCESS DESCRIPTION**

Ethylene (of a purity of or greater than 95%), compressed oxygen and recycle gas are mixed and preheated by product gases from the reactor. An ethylene concentration of 15 - 40 vol% is usually employed. The gas stream enters a tubular reactor containing a silver oxide catalyst supported on a porous carrier (such as aluminium oxide) which has been fired to a high temperature. The fixed-bed catalyst contains 7 - 20% of silver and promoters – compounds of alkalis or alkaline earth metals especially caesium and barium.

Selectivity is improved by the addition of chlorine compounds (such as ethyl chloride or vinyl chloride) which reduce the production of by-product carbon dioxide and ensures an even surface coating. As the activity of the catalyst declines, the reaction temperature is gradually increased to maintain ethylene oxide production. Ethylene and any other gases used must be free from sulphur, sulphur compounds or acetylene which are catalyst poisons. Catalyst life is 2 - 4 years.

The reaction conditions are a temperature 200 - 300°C and pressure of 10 - 30 bar, with a residence time of one second. Small amounts of methane are added as diluent which helps to increase the flammable limit in the reactor. The gas phase reaction is highly exothermic, the oxidation temperature is controlled by boiling water or a high boiling hydrocarbon in an outer reactor jacket to remove the heat produced. Any excess heat is used to generate steam which is circulated to the ethylene oxide recovery section.

The reactor gases are cooled and compressed before passing to a scrubber where chilled water absorbs the ethylene oxide. The dilute aqueous ethylene oxide solution is steam stripped and the resultant ethylene oxide purified by fractionation. Ethylene glycol is

produced as by-product when ethylene oxide comes into contact with water in the scrubber can be recovered from the waste streams.

By-product carbon dioxide in the gases from the top of the scrubber is removed by absorption with hot aqueous potassium carbonate. Steam stripping at atmospheric pressure releases the carbon dioxide which is vented and the potassium carbonate solution is pumped back to the absorber.

A portion of the recycle gas stream from the absorber is removed and flared in order to avoid the build-up of inert gases present in the feed gases.

# **CHAPTER 4**

# **MATERIAL BALANCE**

#### Basis: 100 kmol/hour mixed feed

#### **Assumptions:**

- > 2% of ethylene oxide is converted to ethylene glycol by reacting with water.
- > 5% extra water is used to absorb all of the ethylene oxide fed into the coloumn.
- > Solubility of ethylene oxide is water is  $10^6$  mg/L of water.

Typical values, taken from the literature are cited:

- $\geq$  25% of C<sub>2</sub>H<sub>4</sub> converted to C<sub>2</sub>H<sub>4</sub>O in the reactor
- $\geq$  25% of C<sub>2</sub>H<sub>4</sub> is converted to CO<sub>2</sub> and H<sub>2</sub>O in the reactor
- $\triangleright$  C<sub>2</sub>H<sub>4</sub>: O<sub>2</sub> = 1:10 and 2 kmol inert

Let  $X = C_2H_4$  and  $Y = O_2$ 

10X = Y and X+Y = 98

 $C_2H_4$  in the feed = 98/11 = 8.909 kmol

 $O_2$  in the feed = 89.09 kmol

Single Pass Conversion = 50%

 $C_2$  H<sub>4</sub> in the Feed Stream entering the Reactor,  $n_1 = 4.454$  kmol

 $O_2$  in the feed stream entering the Reactor,  $10n_1 = 44.54$  kmol

Again,

25% of  $C_2H_4$  is converted to ethylene oxide ( $C_2H_4O$ ) and other 25% to  $CO_2$  and  $H_2O$ .

 $C_2H_4+ {}^1\!\!/_2 O_2 \ \rightarrow \ C_2H_4O$ 

 $C_2H_4O+3\ O_2 \rightarrow \ 2CO_2+2\ H_2O$ 

 $n_2 = (8.909*0.25) = 2.227 \text{ kmol } C_2H_40$ 

 $n_3 = (2*8.909*0.25) = 4.454 \text{ kmol } \text{CO}_2$ 

 $n_4 = (2*8.909*0.25) = 4.454 \text{ kmol } H_2O$ 

#### **4.1. BALANCE FOR THE REACTOR**

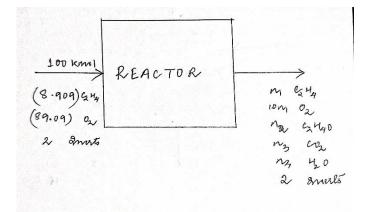


Figure 4.1: Reactor

Table 4.1: Balance over reactor

Input(Kg/hr)	(Kg/hr) Output(Kg/hr)		r)
C <sub>2</sub> H <sub>4</sub>	249.897	C <sub>2</sub> H <sub>4</sub>	124.95
O <sub>2</sub>	2850.7	O <sub>2</sub>	2601.27
Inerts	56	C <sub>2</sub> H <sub>4</sub> O	98.01
		CO <sub>2</sub>	196.04

		H <sub>2</sub> O	80.24
		Inert	56
Total	3156.6	Total	3156.51

 $O_2$  required for  $C_2H_4O$  production= 0.5\*2.227 = 1.1135 kmol/hr = 35.63 kg/hr

 $O_2$  required for ( $CO_2 + H_2O$ ) formation = 3/2 \* 4.454 = 6.681 kmol/hr = 213.8 kg/hr

Accumulation of  $O_2 = (2850.7 - 213.8 - 35.63) = 2601.27 \text{ kg/hr}$ 

#### 4.2. BALANCE OVER THE ETHYLENE OXIDE ABSORBER

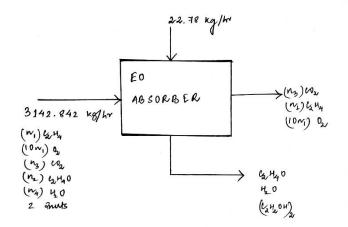


Figure 4.2: Ethylene oxide absorber

Let,

2% of input EO  $(n_2)$  reacted with Water to form ethylene glycol.

Therefore, Ethylene glycol produced = 2% of  $n_2$ 

$$= 2.765 \text{ kg/hr}$$

Other 98% of EO has gone with H<sub>2</sub>O

As aqueous solution of  $EO = 0.98 \times 2.227$ 

= 2.18 kmol/hr = (2.18\*44.05) = 96.16 kg/hr

Total water (H<sub>2</sub>O) input = (80.21 + 22.78) = 102.33 kg/hr = 5.717 kmol/hr

Solubility of EO in water =  $10^6 \text{ mg/L} = 1 \text{kg/L}$ 

$$N_2 = 98.1 \text{ kg/hr}$$

 $C_2H_4O + H_2O \rightarrow (C_2H_2O_4)_2$ 

98.1 kg EO requires 98.1 kg H<sub>2</sub>O to form EG.

Also, 1kg  $\approx$  1L (pure water)

Amount of extra water required = (98.1 - 80.2) 17.9 kg/hr.

But we have assumed 5% of n<sub>4</sub> extra

Therefore,

Amount of water needs to be added = 17.9 + (0.05\*98.1) = 22.78 kg/hr

Now,

 $H_2O$  required for ethylene glycol formation = 0.044 kmol/hr

 $H_2O$  left which is released with EO = (5.717 - 0.044)

= 5.673 kmol/hr

$$= 102.199 \text{ kg/hr}$$

#### Table 4.2. Balance over ethylene oxide Absorber

Input (kg/hr)	Output (kg/hr)
Output from reactor = 3156.597	$C_2H_4O = 96.16$
$H_2O$ added = 22.78	$H_2O = 102.199$
	$CO_2 = 196.04$
	$(C_2H_2O_4)_2 = 2.765$
	$C_2H_4 = 124.95$
	$O_2 = 2601.27$
	Inert = 56
Total = 3179.377	Total = 3179.38

### 4.3. BALANCE OVER CO<sub>2</sub> ABSORBER

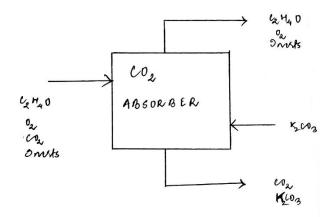


Figure 4.3: CO<sub>2</sub> absorber

According to literature, amount of  $K_2CO_3$  required in the  $CO_2$  absorber is 30% of  $CO_2$ 

 $n_3 = 196.04 \ kg/hr = 58.806 \ kg/hr$ 

And same amount of  $K_2CO_3$  from the  $CO_2$  stripper is fed back to the  $CO_2$  absorber so that there is no loss of  $K_2CO_3$ .

Assuming 100% absorption and no formation of other product, amount of  $K_2CO_3$  in the absorber = amount of  $K_2CO_3$  going out of absorber = 58.806 kg/hr

Input (kg/hr)		Output (kg/hr)	
C <sub>2</sub> H <sub>4</sub>	124.95	$C_2H_4 = 124.95$	124.95
O <sub>2</sub>	2601.27	O <sub>2</sub>	196.04
CO <sub>2</sub>	196.04	CO <sub>2</sub>	58.806
K <sub>2</sub> CO <sub>3</sub>	58.806	K <sub>2</sub> CO <sub>3</sub>	58.806
Inert	56	Inert	56
Total	3037.066	Total	3037.066

Table 4.3. Balance over CO<sub>2</sub> Absorber

## 4.4. BALANCE OVER CO<sub>2</sub> STRIPPER

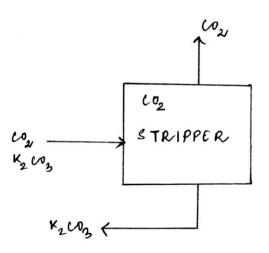


Figure 4.4: CO<sub>2</sub> Stripper

Table 4.4. Balance over CO<sub>2</sub> stripper

Input (kg/hr)	Output (kg/hr)
$CO_2 = 196.04$	CO <sub>2</sub> = 196.04
$K_2CO_3 = 58.806$	$K_2CO_3 = 58.806$
Total = 254.846	Total = 254.846

#### **4.5. BALANCE OVER DISTILLATION COLUMN 1:**

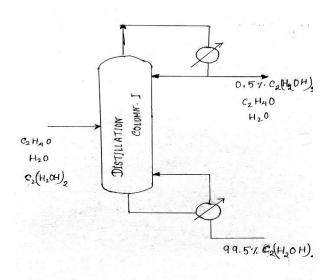


Fig:4.5: Distillation column 1

Assuming 0.6% of ethylene glycol come up with overhead product of distillation column and rest 99.5% goes out as bottom product.

 $(C_2H_2O_4)_2$  in overhead product = 0.5% of 2.765 = 0.014 kg/hr

 $(C_2H_2O_4)_2$  in bottom product = 99.5% of 2.765 = 2.751 kg/hr

## Table 4.5. Balance over Distillation Column 1

Input (kg/hr)	Output (kg/hr)
$C_2H_4O = 96.161$	$C_2H_4O = 96.161$
$H_2O = 102.199$	$H_2O = 102.199$
$(C_2H_2OH)_2 = 2.765$	$(C_2H_2OH)_2$ (overhead) = 0.014
	$(C_2H_2OH)_2$ (bottom) = 2.751
Total = 201.125	Total = 201.125

# 4.6. BALANCE OVER DISTILLATION COLOUMN 2

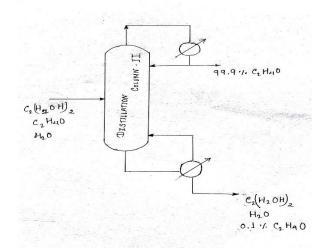


Fig :4.6 Distillation column 2

Feed = kmoles of  $C_2H_4O$  + kmoles of  $H_2O$  + kmoles of  $(C_2H_2OH)_2$ 

= 2.18 + 5.673 + 0.000226

= 7.85 kmoles/hr

 $x_F = 2.18 \; / \; 7.85 = 0.277; \; x_D = 0.999; \; x_W = 0.001$ 

Overall material balance, F = D + W

$$\Rightarrow$$
 7.85 = D+W

Component (ethylene oxide) balance,  $Fx_f = Dx_D + Wx_W$ 

$$\Rightarrow 7.85 \times 0.277 = D \times 0.999 + W \times 0.001$$

Solving these two equations, D = 2.1709 kmol/hr

$$W = 5.679$$
kmol/hr

#### Table 4.6. Balance over Distillation Column 2

Input (kg/hr)		Output (kg/hr)	
C <sub>2</sub> H <sub>4</sub> O	96.161	C <sub>2</sub> H <sub>4</sub> O	0.25+95.628=95.878
H <sub>2</sub> O	102.199	H <sub>2</sub> O	102.199
$(C_2H_2OH)_2$	2.765	(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	2.765
Total	201.125	Total	200.84

Now,

 $n_7 = n_1 + 10n_1 + 2 = 11n_1 + 2 = 50.994$ 

 $x_7 = n_1 \ / \ 50.994 = 0.087$ 

Mole balance,  $n_0 + n_8 = 100$ 

Inert balance,

 $0.005 n_0 + (1 - 11x_7) n_8 = 2$ 

 $=>0.005\ n_0+0.043\ x_8=2$ 

Therefore,

 $n_8 = 60.52, R = n_8 = 39.47$ 

 $n_6 = P = n_7 - R = 11.524 \text{ kmol/hr}_0$ 

### **RECYCLE STREAM COMPOSITION**

 $x_7 = n_1/R = n_1(C_2H_4) = 3.433$ kmol

Inert:  $(1-11x_7) = I/R \Rightarrow I = 1.69$ kmol

## PURGE STREAM COMPOSITION

 $x_7 = n_1/P \Rightarrow$   $n_1 (C_2H_4) = 1.0025 \text{kmol}$ 

Inert,  $(1-11x_7) = I/P \Rightarrow I = 0.4955$ kmol

## FRESH FEED COMPOSITION

Here,  $n_0 = 60.52$ , Inert in the feed stream = 0.5% of  $n_0 = 0.3026$ 

 $n_0 - inert = 60.217$ 

$$\Rightarrow$$
 Moles of (C<sub>2</sub>H<sub>4</sub>+O<sub>2</sub>) = 60.217 & & 10C<sub>2</sub>H<sub>4</sub> = O<sub>2</sub>

Moles of  $C_2H_4$ = 5.47 kmol and Moles of  $O_2$ = 54.743 kmol

### **INERT BALANCE**

In the feed stream =  $0.5/100 \times 60.52 = 0.3026$  kmol/hr

In the purge stream =  $(1-11x_7) \times P = 0.395$ kmol/hr

# CHAPTER 5

# **MODIFIED MATERIAL BALANCE**

Selected production capacity = 10,000 ton/annum

No. Of working days = 330 days

Production rate in Kg/hr = 1262.626 Kg/hr

Fresh feed = 86.956Kmol/hr = 2749.201 Kg/hr

Scale Up Factor = 1262.626/2749.201 = 0.459

## Table 5.1. Balance over Reactor

Inp	Input(kg/hr)		tput(kg/hr)
C <sub>2</sub> H <sub>4</sub>	114.7	C <sub>2</sub> H <sub>4</sub>	57.35
O <sub>2</sub>	1308.47	O <sub>2</sub>	1193.98
Inerts	25.70	C <sub>2</sub> H <sub>4</sub> O	45.02
		CO <sub>2</sub>	89.98
		H <sub>2</sub> O	36.83
		Inert	25.70
Total	1448.87	Total	1448.86

# Table 5.2. Balance over Ethylene Oxide Absorber

Input (kg/hr)		Output (kg/hr)	
Output from the	1448.88	C <sub>2</sub> H <sub>4</sub> O	44.14
reactor			
H <sub>2</sub> O added	10.46	H <sub>2</sub> O	46.91
		C <sub>2</sub> O	89.98
		(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	1.27
		C <sub>2</sub> H <sub>4</sub>	57.35
		O <sub>2</sub>	1193.98
		Inert	25.70
Total	1459.34	Total	1459.33

# Table 5.3. Balance over Carbon Dioxide Absorber

Input (kg/hr)		Output (kg/hr	)
C <sub>2</sub> H <sub>4</sub>	57.35	C <sub>2</sub> H <sub>4</sub>	57.35
O <sub>2</sub>	1193.98	O <sub>2</sub>	1193.98
Inert	25.70	Inert	25.70
CO <sub>2</sub>	89.98	CO <sub>2</sub>	89.98
K <sub>2</sub> CO <sub>3</sub>	26.99	K <sub>2</sub> CO <sub>3</sub>	26.99
Total	1394	Total	1394

# Table 5.4. Balance over Carbon Dioxide Stripper

Input (kg/hr)	Output (kg/hr)

CO <sub>2</sub>	89.98	CO <sub>2</sub>	89.98
K <sub>2</sub> CO <sub>3</sub>	26.99	K <sub>2</sub> CO <sub>3</sub>	26.99
Total	116.97	Total	116.97

# Table 5.5. Balance over Distillation Column 1

Input (kg/hr)		Output (kg/hr)	Output (kg/hr)		
C <sub>2</sub> H <sub>4</sub> O	44.15	C <sub>2</sub> H <sub>4</sub> O	44.15		
H <sub>2</sub> O	46.91	H <sub>2</sub> O	46.91		
(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	1.27	(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub> (Enriched)	0.006426		
		(C <sub>2</sub> H <sub>2</sub> OH) (Bottom product)	1.26		
Total	92.33	Total	92.32		

# Table 5.6. Balance over Distillation Column 2

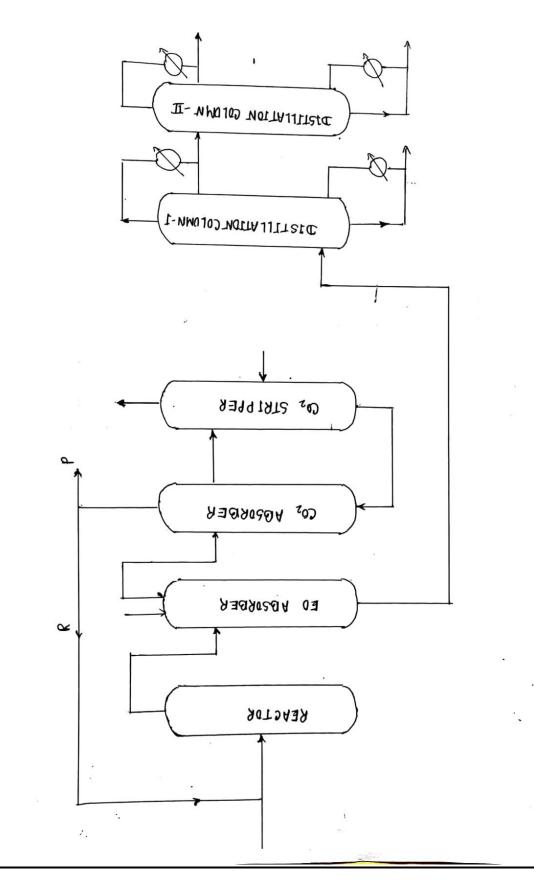
Input (kg/hr)		Output (kg/hr)	Output (kg/hr)	
C <sub>2</sub> H <sub>4</sub> O	44.15	C <sub>2</sub> H <sub>4</sub> O	44	
H <sub>2</sub> O	47.27	H <sub>2</sub> O	47.27	
(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	1.27	(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	1.27	
Total	92.69	Total	92.54	

# 5.1. OVERALL MATERIAL BALANCE

# Table 5.7: Overall balance

INPUT			OUTPUT				
COMPONEN	Mol Wt.	Moles	Amoun	COMPONEN	Mol	Moles(	Amoun
Т	(g/mol)	(Kmo	t	Т	wt(g/mol	Kmol/h	t(Kg/hr
		l/hr)	(Kg/hr)		)	r)	)
C <sub>2</sub> H <sub>4</sub>	28.05	2.1	70.43	C <sub>2</sub> H <sub>4</sub> O	44.05	0.998	44
O <sub>2</sub>	15.99	25.13	401.78	H <sub>2</sub> O	18.015	2.62	47.27
INERTS	14.00	0.14	1.94	(C <sub>2</sub> H <sub>2</sub> OH) <sub>2</sub>	62.07	0.02	1.27
				C <sub>2</sub> H <sub>4</sub>	28.05	0.46	12.9
				O <sub>2</sub>	15.99	4.6	323.58
				INERTS	14.00	0.227	3.18
Total = 474.15 kg/hr				T	otal= 473.	65 kg/hr	

# **FLOWSHEET**



# CHAPTER 6

# **ENERGY BALANCE**

### 6.1 Energy balance over REACTOR

### **INPUT TO THE REACTOR**

 $C_2H_4 = 114.70 \text{ kg/hr} = 4.096 \text{ kmol/hr}$ 

 $O_2 = 1308.47 \text{ kg/hr} = 40.9 \text{ kmol/hr}$ 

Inerts = 25.70 kg/hr = 0.918 kmol/hr

TOTAL = 1448.87 kg/hr=45.914kmol/hr

#### **OUTPUT TO THE REACTOR**

 $C_2H_4 = 57.35 \ kg/hr = 2.048 \ kmol/hr$ 

 $O_2 = 1193.98 \text{ kg/hr} = 37.31 \text{ kmol/hr}$ 

 $C_2H_4O = 45.03 \text{ kg/hr} = 1.023 \text{ kmol/hr}$ 

 $CO_2 = 89.98 \text{ kg/hr} = 2.045 \text{ kmol/hr}$ 

 $H_20 = 36.83 \text{ kg/hr} = 2.046 \text{ kmol/hr}$ 

Inerts = 25.70 kg/hr = 0.918 kmol/hr

TOTAL = 1448.87 kg/hr=46.413kmol/hr

 $T_{ref} = 25^{\circ}C$  (datum temperature)

Considering feed entering at 25° °C

Reaction temperature  $T_R = 280$ °C

Table 6.1: Heat capacity data for products and unreacted reactants at 280°C

Component	Cp (J/kgK)	
C <sub>2</sub> H <sub>4</sub> O	1714.54	
C <sub>2</sub> H <sub>4</sub>	2409.25	
O <sub>2</sub>	988.3	
N <sub>2</sub>	1065.6	
CO <sub>2</sub>	1046.884	
H <sub>2</sub> O	1858	

The two reactions taking place in this process are given below:

## Main reaction:

 $C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O; \Delta H^{\circ}_{298.15} = -106.7 \text{ kJ/mol}$ 

### Side reaction:

 $C_2H_4O + 3O_2 \rightarrow \qquad 2CO_2 + 2H_2O; \Delta \quad {}^{_{H^\circ}_{_{298.15}}} = \text{-} \ 1323 \text{ kJ/mol}$ 

## **ENERGY BALANCE EQUATION FOR THE REACTOR:**

 $m \; Cp \Delta \quad T \; {}_{reactants} + Q \; {}_{heat \; removed \; by \; exothermic \; reaction} + \Delta \qquad H_R = m \; Cp \Delta \qquad T \; {}_{products}$ 

For reactants,

 $\Delta T = (25-25) = 0^{\circ}C$ 

m Cp  $\Delta$  T <sub>reactants</sub> = 0

 $T_P = 280^{\circ}C$  and  $T_R = 25^{\circ}C$ 

 $m\;Cp\;\Delta \;T_{\;products}$ 

 $= [(mCp)_{E} + (mCp)_{O2} + (mCp)_{EO} + (mCp)_{CO2} + (mCp)_{Inerts} + (mCp)_{H2O}] (T_{P} - T_{R})$ 

 $= 1.333 * 10^8$  Joules

# HEAT OF THE REACTION (at 280° °C)

where,

$C_p$	=	heat	capacity	(J/mol*K)
H°	=	standard	enthalpy	(kJ/mol)
t = temp	perature (K) / 10	00		

Data from NIST web book:

Components	А	В	С	D	E	F	G
C <sub>2</sub> H <sub>4</sub>	-6.38	184.40	-112.97	28.49	0.31	48.17	52.46
O <sub>2</sub>	31.32	-20.23	57.86	-36.50	-0.007	-8.90	0
C <sub>2</sub> H <sub>4</sub> O	-23.36	275.7	-188.97	51.03	0.39	28.17	-163.16
CO <sub>2</sub>	24.99	55.20	-33.70	7.95	-0.14	-403.60	-393.50
H <sub>2</sub> 0	-203.60	1523.29	-3196.4	2474.50	3.86	-256.50	-285.80

For main reaction

 $C_2H4 + \frac{1}{2}O_2 \rightarrow C_2H_4O; \Delta H^{\circ}_{298} = -106.7 \text{ kJ/mol}$ 

Now,

 $A = A(C_2H_4O) - A(C_2H_4) - 0.5A(O_2) = -32.54$ 

Similarly,

B = 101.415 C = -104.93 D = 40.79 E = 0.0835 F = 4.45 G = -215.62Therefore, from equation (i), At 298K

 $H^{\circ}_{298.15} = 7.948 * 10^{10}$  Joules

At 553K,

 $_{\text{H}^{\circ}} = 8.686 * 10^{11}$  Joules

But since conversion is only 25%

Therefore,  $^{H_{\circ}} = (8.686 * 10^{11}) * 0.25 * 4.096 = 8.894 * 10^{11}$  Joules

Similarly for side reaction,

 $C_2H_4O + 3O_2 \rightarrow 2CO_2 + 2H_2O; H^{\circ}_{298.15} = -1323 \text{ kJ/mol}$ 

 $A = 2A(C_2O) + 2A(H_2O) - A(C_2H_4O) - 3A(O_2) = -444.73$ 

Similarly,

B = 3033.18

C = -6520.93

D = 5045.90 E = 7.145 F = -1341.70 G = -1411.1 Therefore, from equation (i), At 298K

 $H^{\circ}_{298.15} = 9.89 * 10^{12}$  Joules

At 553K,

 $H^{\circ} = 1.077 * 1014$  Joules

But since conversion is only 25%

Therefore,  $H^{\circ} = (1.077 * 10^{14}) * 0.25 * 4.096 = 1.1 * 10^{14}$  Joules

Heat removed =  $(1.1 * 10^{14} - 1.333 * 10^8)$  Joules =  $1.099 * 10^{14}$  Joules

Boiling water is used for removal of heat,

m Cp  $\Delta$  T <sub>water</sub> = 1.099 \* 10<sup>14</sup> Joules

 $= m_{\text{water}} = (1.099 * 10^{14})/(4180 * (90 - 25)) = 4.044 * 10^8 \text{ kg}$ 

## 6.2 ENERGY BALANCE FOR THE HEAT EXCHANGER

In the heat exchanger the product vapours are cooled from 280° °C to 35°C. The removed energy is supplied to the recycle stream.

#### Table 6.3. Cp values at temperature 35°C

Component	Cp (J/kgK)	
C <sub>2</sub> H <sub>4</sub> O	1120.95	
C <sub>2</sub> H <sub>4</sub>	1769.14	
O <sub>2</sub>	918.52	
N <sub>2</sub>	1040	
CO <sub>2</sub>	858.23	
H <sub>2</sub> O	4180	

 $T_P=35^{\circ}\text{C} \qquad \text{ and } \quad T_R=25^{\circ}\text{C}$ 

 $m \; Cp \Delta \qquad T \; {}_{products \; leaving \; the \; heat \; exchanger}$ 

 $= [(mCp)_{E} + (mCp)_{O2} + (mCp)_{EO} + (mCp)_{CO2} + (mCp)_{Inerts} + (mCp)_{H2O}] (T_{P} - T_{R})$ 

 $= 1.505 * 10^7$  Joules

m Cp $\Delta$  T products entering the heat exchanger =  $1.333 * 10^8$  Joules

Heat removed in the exchanger =  $(1.33 \times 10^8 - 1.505 \times 10^7) = 1.18 \times 10^8$  Joules

## **6.3 ENERGY BALANCE IN THE COMPRESSOR**

# Table 6.4. Density and mole fraction of the components

Components	Density (kg/m <sup>3</sup> )	Mole fraction (x)
C <sub>2</sub> H <sub>4</sub> O	851.61	0.0225
C <sub>2</sub> H <sub>4</sub>	212.21	0.045
O <sub>2</sub>	435.36	0.822
N <sub>2</sub>	464.64	0.045

CO <sub>2</sub>	314.076	0.02
H <sub>2</sub> O	993.719	0.045

Average density

 $= [(\rho \ x)_{\rm E} + (\rho \ x)_{\rm O2} + (\rho \ x)_{\rm EO} + (\rho \ x)_{\rm CO2} + (\rho \ x)_{\rm Inert} + (\rho \ x)_{\rm H2O}] = 458.48 \ \text{kg/m}^3$ 

 $\rho = m/V$ 

 $=> V = m/\rho = 3.16 \text{ m}^3$ 

Work required in the compressor to increase the pressure from 5 to 10 atm

 $W = V * (P_2 - P_1) = 1.6 * 10^6 J$ 

This work will be added to the enthalpy

= ( $1.505 * 10^7 - 1.6 * 10^6$ ) J =  $1.346 * 10^7$  J

Therefore, energy leaving the compressor =  $1.346 * 10^7 \text{ J}$ 

## 6.4 ENERGY BALANCE FOR THE ETHYLENE OXIDE ABSORBER

In the EO absorber, the ethylene oxide is completely absorbed in the water at 25°C.

Only the energy is lost from the gases which are not absorbed in the absorbing liquid.

Energy entering the absorber =  $1.346 * 10^7 \text{ J}$ 

Output from the absorber

 $C_2H_4 = 57.35 \text{ kg/hr} = 2.048 \text{ kmol/hr}$ 

 $O_2 = 1193.98 \text{ kg/hr} = 37.31 \text{ kmol/hr}$ 

 $C_2H_4O = 45.03 \text{ kg/hr} = 1.023 \text{ kmol/hr}$ 

 $CO_2 = 89.98 \text{ kg/hr} = 2.045 \text{ kmol/hr}$ 

 $H_20 = 36.83 \text{ kg/hr} = 2.046 \text{ kmol/hr}$ 

Inert = 25.70 kg/hr = 0.918 kmol/hr

Energy lost from the absorber

 $= [(mCp)_{E} + (mCp)_{O2} + (mCp)_{EO} + (mCp)_{CO2} + (mCp)_{Inerts}] = 1.35 * 10^{6} \text{ J}$ 

Therefore,

Energy leaving the absorber with the product =  $(1.346 * 10^7 - 1.35 * 10^6) = 1.211 * 10^7$ J

### 6.5 ENERGY BALANCE FOR CARBON DIOXIDE ABSORBER

Energy entering the carbon dioxide absorber at  $25^{\circ}$ C =  $1.211 \times 10^7$  J

Energy lost from the absorber =  $[(mCp)_E + (mCp)_{O2} + (mCp)_{CO2}] \Delta T = 1.28 * 10^6 \text{ J}$ 

Energy leaving the absorber =  $1.211*101.08 * 10^7 \text{ J}$ 

Energy leaving the absorber with recycle stream =  $3.34 * 10^8$  J

#### 6.6 ENERGY BALANCE FOR CARBON DIOXIDE STRIPPER

Here the stripper is a steam stripper and it is done at 100°C

Energy entering the stripper =  $1.28 * 10^6$  J at 25°C

Energy leaving the stripper =  $196.04 * 1046.884 * (100 - 25) = 1.539 * 10^7 \text{ J}$ 

## 6.7 ENERGY BALANCE FOR DISTILLATION COLOUMN 1

Enthalpy of the feed to the distillation column,  $H_F = 1.539 \times 10^7$ 

Temperature of the feed=  $35^{\circ}C$ 

For the Column Operating Temperature:

1.Pressure Data:

Bubble Point Pressure: 10bar= 100kPa

Dew Point Pressure:10.5bar= 1050kPa

2. Vapour Pressure equation constants:

Using Antoine Equation,  $\ln P = A-B/(T+C)$ 

Table 6.5. The Antoine Equation for each component

Component	Α	В	С
Ethylene oxide	4.386	1115.1	-29.015
Ethylene Glycol	4.97012	1912.951	-84.996
Water	5.40221	1838.675	-31.737

Bubble point: For bubble point calculation, vapor composition and temperature is

required which is calculated from the formula as:

$$Ki = P_i^{sat} / P$$

Where P<sub>i</sub><sup>sat</sup> is calculated from the Antoine Equation and

$$A_i = K_i/K_c$$

Where  $\alpha_i$  is the relative volatility

K<sub>c</sub> is the base K<sub>i</sub> value (water).

From the calculation performed, bubble point is  $T_{bp}$ = 185°C.

Dew point: Formulas used to obtain dew point temperature is same as bubble point. From the calculation performed, dew point temperature is:  $T_{dp} = 86^{\circ}C$ 

Enthalpy feed to the distillation column =  $1.539 \times 10^7 \text{ J}$ 

Temperature of the feed =  $25^{\circ}C$ 

Enthalpy of gas =  $y_{EO} * [Cp_{EO} * M_{EO} * (T_G - T_F) + LAMDA_{EO}] + y_{H2O} * [Cp_{H2O} + Cp_{H2O} +$ 

 $*M_{H2O} *(T_G - T_F) + LAMDA H2O]$ 

=47423.5 Kj/kmol

 $H_G = 4.7 * 10^7 J$ 

Cooling water required in the condenser =  $M^*Cp^*\Delta T = 4.7^*10^7$ 

Water is getting cooled from 185 to 25° C

Thus M= $4.7 \times 10^7 / (4180 \times 160) = 70.275 \text{ kg/hr}$ 

 $H_{D}=y_{EO}\times[Cp_{EO}\times\Delta T]+y_{H2O}[Cp_{H2O}\Delta T]+y_{EG}[Cp_{EG}\Delta T]=5.47\times10^{5}J$ 

Condenser Duty=  $H_G$  - $H_{Lo}$  - $H_D$ = 4.59×10<sup>7</sup>J

Enthalpy of the Residue,  $H_w = 3600.33 \times 4.18 \times (185-25) = 2.4079 \times 10^6 J$ 

D=199.742kg/hr W=2.75kg/hr

Reboiler Duty=  $199.742 \times 5.47 \times 10^5 + 2.75 \times 2.0479 \times 10^6 - 201.495 \times 1.539 \times 10^7$ 

 $+4.59 \times 10^7 \text{ J}$ 

 $=9.02910^9$ J

#### 6.8 ENERGY BALANCE OVER DISTILLATION COLUMN 2:

Enthalpy of the feed to the distillation column= $5.47 \times 10^5 \text{J}$ 

Temperature of the feed=  $35^{\circ}C$ 

For the Distillation Column,

Bubble Point=55°C Dew Point=93°C

Enthalpy of the gas= $y_{EO}*[Cp_{EO}*M_{EO}*(T_G-T_F) + \lambda_{EO}] + y_{H2O}*[Cp_{H2O}*M_{H2O}]$ 

 $*(T_G - T_F) + \lambda_{H2O}] + y_{C2H6O2} * [Cp_{C2H6O2} * M_{C2H6O2} * (T_G - T_F) + \lambda_{C2H6O2}$ 

]=37942.4KJ/Kmol

 $H_G=1.427 \times 10^7 J$ 

Cooling water is required in the cooler=  $M^*Cp^*\Delta T$ 

 $\Rightarrow \Rightarrow M=13.65$ kg/hr

 $H_{D} = y_{EO}[Cp_{EO} M_{EO} \Delta T] + y_{H2O}[Cp_{H2O} M_{H2O} \Delta T] + y_{EG}[Cp_{EG} \Delta T] = 39030.64 J$ 

 $H_{Lo=}\,39030.64J$ 

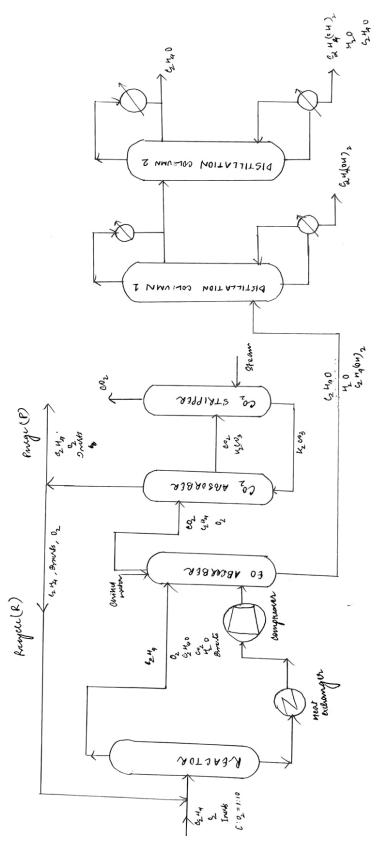
Condenser Duty=  $H_G$ - $H_{Lo}$ - $H_D$ =1.35×10<sup>6</sup>J

Enthalpy of the Residue,  $H_W=3.01\times10^5 J$ 

D=2.1709Kmol/hr, W=5.679Kmol/hr

Reboiler Duty,  $Q_B=D \times H_D+W \times H_W-F \times H_F+Q_C=1.17 \times 10^7 J$ 

# **FLOWSHEET**



## CHAPTER 7

# **DESIGN OF EQUIPMENT**

### 7.1 DESIGN OF PRESSURE VESSEL

#### 7.1.1. Determination of plate thickness for a spherical shell:

Assumptions:

- (i) Class 2 duty operation
- (ii) Material of Construction: Stainless steel IS: 2002-1962 Grade 2B
- (iii) Joint specification: Double welded butt joint
- (iv) Maximum operating pressure: 7 bar  $(7.14 \text{ kgf/cm}^2)$
- (v) Nominal diameter: 1.2 meter

Let thickness = t mm

For spherical vessel,  $t = \frac{PDo}{400 f J + P}$ 

Where,

 $P = Design pressure = 1.05 * 7.14 = 7.49 \text{ kgf/cm}^2$ 

 $D_0$  = Nominal diameter of the shell = 1.2 m = 1200 mm

f=Allowable stress value = 1.18 \*  $10^8~\text{N/m}^2$  (at 250°C )  $~=12.03~\text{kgf/mm}^2$ 

J = Joint factor = 0.85

t = (1200 \* 7.49) / [(400 \* 12.03 \* 0.85) + 7.49] = 3.19 mm

For stainless steel, the corrosion allowance, C = 0

# 7.1.2. Determination of the plate thickness of a compensated standard dished

#### head

Assumptions:

- (i) Material of Construction: Stainless steel IS: 2002-1962 Grade 2B
- (ii) Maximum operating pressure: 7 bar  $(7.14 \text{ kgf/cm}^2)$
- (iii) Nominal diameter(D<sub>0</sub>): 1.2 meter
- (iv)  $R_0 = R_i = D_0 = 1.2$  meter
- (v)  $r_0 = (0.06 * nominal diameter)$

For standard dished head,  $t = \frac{PD_0C}{200fJ}$ 

$$P = 7.49 \text{ kgf/cm}^2$$

$$f = 1.18 * 10^8 \text{ N/m}^2 = 12.03 \text{ kgf/mm}^2$$

#### $D_0 = 1.2 \text{ m}$

As the diameter of the vessel (1.2 m) is not very large head can be fabricated from a single plate and therefore, J = 1.

Hence,

 $\frac{t}{D_0 C} = \frac{P}{200 fJ} = \frac{7.49}{200 \cdot 12.03 \cdot 0.01 \cdot 1} = 0.005$ 

For the effective external height of the head,  $h_E$ :

$$h_0 = R_0 - \sqrt{(R_0 - D_0^2)(R_0 + D_0^2 - 2r_0)} = 0.203 \text{ m}$$

$$\frac{D_0^2}{4R_0} = 0.3 \text{ m}$$
  
 $\sqrt{\left(\frac{D_0 r_0}{2}\right)} = 0.207 \text{ m}$ 

Out of the three quantities calculated above,  $h_0$  is the least. Therefore,  $h_E = 0.203$  m Now,

$$\frac{h_E}{D_0} = \frac{0.203}{1.2} = 0.17$$

With the help of Table 4.1 (A), various values of  $\frac{t}{(D_0 c)}$  are to be tried for  $\frac{h_E}{D_0} = 0.17$  to match the above relationship. It is found that value of C = 1.91 gives  $\frac{t}{D_0 c} = 0.005$  which is a very good approximation. An exact value may be obtained by plotting against C.

From table 4.1 (A), C = 1.91

$$\frac{t}{D_0 c} = 0.005$$
  
=> $\frac{t}{D_0} = 9.55 * 10^{-3} \text{ cm}$ 

$$\Rightarrow$$
 t = 0.011 m

It is to be noted here that for the thinning of the torus no extra allowance is provided.

If 6% allowance is given, thinning allowance = 6%

 $t_s = 0.0116 \ m = 11.6 \ mm$ 

Standard thickness of head,  $t_{std} = 12 \text{ mm}$ 

#### 7.2. DESIGN OF HEAT EXCHANGER

Step 1: LMTD C	Calculation
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 $\Delta T_1 = 160^{\circ}$ C and  $\Delta T_2 = 15^{\circ}$ C

 $\Delta T_{LM} = 61.25^{\circ}C$ 

 $Q_{water} = m Cp = 1.33 * 10^8 J = m * 4184 * (120 - 25)$ 

=> m = 335.36 kg/hr

$$A = \frac{Q}{U_D \Delta T} = 3829.6 \text{ m}^2 = 41201.22 \text{ ft}^2$$

 $Q_{mix} = 1.15 * 10^8 \text{ J} = m * 4184 * (120 - 20)$ 

=> m = 27.48 kg/hr

Therefore, A =  $33.11 \text{ m}^2 = 356.21 \text{ ft}^2 > 200 \text{ ft}^2$ 

 $Q_{h} = 1090.2$  J, Cp = 56.23 J/mol K \*  $\frac{1}{35.583} = 2000.83$  J/kg K

 $Cp_h = 56.29 \text{ J/kg K} = 1.58 \text{ J/kg K} = 0.2936 \text{ Btu/hr }^\circ R$ 

 $Cp_{c water} = 1$ 

 $Q_c = m Cp_c \Delta t = 27.48 * 1* (120 - 20) = 2748 J$ 

Step 2: LMTD = 61.25°C

R = 2.45 and S = 0.385

 $F_{T} = 0.95$ 

 $\Delta T_L = 61.25 * 0.95 = 58.1875^{\circ}C$ 

Step 3: T<sub>cal</sub> or T<sub>av</sub>

 $\Delta T = 160 > 50^{\circ}F \quad \Delta T = 15^{\circ}F$ 

So caloric temperature is used,

 $\Delta T = 280 - 35 = 245^{\circ}C$ 

Specific gravity of mixture

 $= \left[ (0.039*0.974) + (0.324*1.104) + (0.031*0.882) + (0.069*29) + (0.025*1) + \right]$ 

(0.017\*12.5)] = 1.1012

$$^{\circ}API = \frac{141.5}{sp. \ gravity} - 131.5$$

But  $\,^{\circ}$  API come less than 10  $^{\circ}$  API so it is not possible to calculate caloric

temperature.

Average Temperature is used

 $T_{av} = 157.5^{\circ}F$  and  $t_{av} = 70^{\circ}F$ 

## **Table 7.1. Fluid properties**

Mixture (157.5°F)	Cold water (70°F)
$\mu = 0.012 * 2.42 = 0.029 $ lb/ft.hr	$\mu = 1.08 * 2.42 = 2.6136 \text{ lb/ft.hr}$
$Cp = 1.580 \text{ btu/lb.}^\circ \text{F}$	Cp = 1 btu/lb.° F
$K = 0.423 \text{ btu/hr.ft}^2(^{\circ} \text{ F/ft})$	K = 0.3497
S = 1.1012 * 62.5 = 68.825	S = 1 = 62.5

Positioning of streams

$$2 1\frac{1}{4}$$
, ID,  $\frac{3}{4}$ , OD, 16' long, 1" sq pitch, B = 5

ID = 21.25 in, 
$$P_T = 1$$
  
C' =  $P_T - OD = 0.25$ "  
 $a_s = \frac{ID \times c' \times B}{144 P_T} = 0.184 \text{ ft}^2$   
 $a_t = \frac{N_t \times a'_t}{144 n} = 0.1678 \text{ ft}^2$  (at" = 0.302 from table 10)

Water goes on tube side and the mixture goes on shell side.

# Table 7.2. For calculation of heat transfer coefficient

Shell side (mixture)	Tube side (water)
$a_s = 0.184 \text{ ft}^2$	$a_t = 0.1678 \ ft^2$
$G_s = 1002.316 \text{ lb/hr ft}^2$	$G_t = 1995.104 \text{ lb/hr ft}^2$
$D_e = 0.95^{"} = 0.0791^{"}$	ID = 0.620" = 0.0516'
$Re_s = 6606.93$	$Re_t = 393.398$
j <sub>H</sub> = 44	$v = 1.25 * 10^{-3}$
$h_0 = 83.58$	$h_i = 400 \text{ Btu/hr}$
	Correction factor =0.98
	$h_i = 392 \text{ Btu/hr}$

 $h_{i0}=h_i*\frac{{\it ID}}{{\it OD}}=324.05~Btu/hr$ 

Clean overall coefficient  $U_c = \frac{h_{i0}h_i}{h_{i0}+h_i} = 66.44$ 

 $a'' = 0.1963 \ lin \ ft, \ ft^2$ 

 $A = 16 * 0.1963 * 160 = 502.528 \text{ ft}^2$ 

$$U_{\rm D} = \frac{Q}{A\Delta T} = 37.36$$

Table 7.3. Pressure drop

Shell side	Tube side
$Re_s = 6606.93$	$Re_t = 393.398$
$f = 0.0003 \ ft^2/m^2$	$f = 0.0038 \text{ ft}^2/\text{m}^2$
$N + 1 = \frac{12L}{B} = 38.4$	$\Delta P_t = \frac{f G_t^2 D_s Ln}{5.22 \times 10^{10} \times Di \times \rho} = 1.79 \text{ psi}$
$D_e = 21.25$ " = 1.77'	$\Delta P_r = \frac{4nv^2}{s \times 2g} = 2.64 \text{ psi}$
$\Delta P_{s} = \frac{f G_{s}^{2} D_{s}(N+1)}{5.22 \times 10^{10} \times D e \times \rho} = 4.5 \text{ psi}$	$\Delta P_T = \Delta P_t + \Delta P_r = 4.439 \text{ psi}$

# **CONCLUSION**

Ethylene oxide is toxic and a potential human carcinogen. Its vapour is extremely irritating to eyes, causing permanent damage, and to the respiratory tract. Exposure can cause headaches, nausea, damage to lungs and finally coma and death. In contact with skin, blisters are formed and absorption takes place.

In this project, our objective was to study the development and designing of the complete process and also the equipment used. Proper raw material, optimum efficiency, safety and economy of the plant have also been looked into.

In performing this project, we have calculated the capacity of a pressure vessel to store the ethylene oxide for 30 days.

In course of our project, we have studied starting from the various available process factors like raw materials, safety, economy, efficiency etc. A suitable process was selected to serve our desired purpose in an economical way. A complete material balance and energy balance of the whole process and in each of the equipment is done in a comprehensive manner.

The project has helped us in great way in acquiring good knowledge of the practical problems that a chemical engineer must face while designing a practical plant.

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