MANUFACTURE OF ETHYLENE OXIDE

MAYANK JYOTI GOHAIN
SHIMANTA KALITA
MAYURAKHI DEB
SOMIMA AKTAR

DEPARTMENT OF CHEMICAL ENGINEERING
ASSAM ENGINEERING COLLEGE,
GUWAHATI-781013

JUNE 2024

MANUFACTURE OF ETHYLENE OXIDE

EIGHTH SEMESTER B.Tech PROJECT

Submitted in partial fulfillment of
The Requirements for the Degree of

BACHELOR OF TECHNOLOGY
in
CHEMICAL ENGINEERING
of
ASSAM SCIENCE AND TECHNOLOGY UNIVERSITY
by

MAYANK JYOTI GOHAIN (200610010028)
SHIMANTA KALITA (212350010005)
MAYURAKHI DEB (200610010029)
SOMIMA AKTAR (200610010049)

DEPARTMENT OF CHEMICAL ENGINEERING
ASSAM ENGINEERING COLLEGE,
GUWAHATI-781013

JUNE 2024

CERTIFICATE FROM THE SUPERVISOR

This is to certify that the project “Manufacture of Ethylene Oxide” has been carried out and presented by:

1. MAYANK JYOTI GOHAIN (200610010028)
2. SHIMANTA KALITA (212350010005)
3. MAYURAKHI DEB (200610010029)
4. SOMIMA AKTAR (200610010049)

Students of 8th semester (Chemical Engineering), Assam Engineering College, under my supervision and guidance in a manner satisfactory to warrant its acceptance as a prerequisite for the award of the degree of Bachelor of Technology in Chemical Engineering of Assam Science & Technology University.

Further, the report has not been submitted/ reproduced in any form for the award of any other degree/ Diploma.

Date:

Place: Guwahati

Dr. Kabita Chakrabarty
Department of Chemical Engineering

Mousumee Das
Department of Chemical Engineering
Assam Engineering College
Jalukbari, Guwahati- 781013

CERTIFICATE FROM THE HEAD OF THE DEPARTMENT

This is to certify that the project entitled "Manufacturing of Ethylene Oxide" has been submitted by the following B.Tech. 8th semester students:

1. MAYANK JYOTI GOHAIN (200610010028)
2. MAYURAKHI DEB (200610010029)
3. SHIMANTA KALITA (212350010005)
4. SOMIMA AKTAR (200610010049)

In fulfilment of the requirements for the award of the degree of Bachelor of Technology in Electrical Engineering of Assam Science & Technology University.

Date:

Dr. Bandana Chakrabarty
Head of the Department
Department of Chemical Engineering
Assam Engineering College

DECLARATION

Report Title: Production of Ethylene Oxide

Degree for which the report is submitted: Bachelor of Technology (Chemical Engineering)

We declare that the presented report represents largely our own ideas and work in our own words. Where other's ideas or words have been included, we have adequately cited and listed in the reference of this report. This report has been prepared following all the principles of academic honesty and integrity. No falsified or fabricated data have been presented in this report. All information contained in this report is correct to the best of our knowledge.

Date:

NAME	ASTU ROLL.NO	SIGNATURES
MAYANK JYOTI GOHAIN	(200610010028)	
SHIMANTA KALITA	(212350010005)	
MAYURAKHI DEB	(200610010029)	
SOMIMA AKTAR	(200610010049)	

ACKNOWLEDGEMENT

It is our privilege to express our sincerest regards to our project Guide Dr. Kabita Chakrabarty And Mousumee Das ma'am for their valuable inputs, able guidance, encouragement, whole-hearted cooperation and constructive criticism throughout the duration of our project.

We deeply express our sincere thanks to our Head of Department Dr Bandana Chakrabarty ma'am for encouraging and allowing us to present the project on the topic "Manufacture of Ethylene oxide" at our department premises for the fulfilment of the requirements leading to the award of B-Tech degree.

We take this opportunity to thank all our lecturers who have directly or indirectly helped our project. Last but not the least we express our thanks to our friends for their cooperation and support.

MAYANK JYOTI GOHAIN	(200610010028)
SHIMANTA KALITA	(212350010005)
MAYURAKHI DEB	(200610010029)
SOMIMA AKTAR	(200610010049)

PROJECT AT A GLANCE

This report details the manufacturing process of ethylene oxide (EO) via the direct oxidation method, utilizing ethene as the primary raw material. Ethylene oxide is a vital industrial chemical, extensively used in the production of ethylene glycol, detergents, and as a sterilizing agent. The direct oxidation process involves the reaction of ethene with oxygen under controlled temperature and pressure conditions. This method is preferred for its efficiency and relatively lower environmental impact compared to alternative routes.

Capacity of the plant: 45000TPA (of Ethylene Oxide)

Ethylene input to the process: 11415.37 kg/hr

Oxygen input to the process: 24681.888 kg/hr

Ethylene Oxide output from the process: 5680.75 kg/hr

Overall material input to the plant: 117341.81 kg/hr

Overall material output from the plant: 117341.81 kg/hr

Overall energy input to the plant: 6256.98 KJ/mol

Overall energy output from the plant: 621.14 KJ/mol

TABLE OF CONTENTS

LIST OF FIGURES AND TABLES

CHAPTER 1: INTRODUCTION

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. Ethylene oxide is a colorless and flammable gas with a faintly sweet odor. Because it is a strained ring, ethylene oxide easily participates in a number of addition reactions that result in ring-opening. Ethylene oxide is isomeric with acetaldehyde and with vinyl alcohol. Ethylene oxide is industrially produced by oxidation of ethylene in the presence of silver catalyst.

Ethylene oxide also helps manufacture medications that better deliver needed treatments to patients. End-use products ranging from fungicides to safety glass are made using ethylene oxide. Ethylene oxide is used to make a variety of products found all around your house from shampoos to disinfectants to laundry detergent. It is also a necessary ingredient for some highly durable fabrics and textiles used in clothing, carpet, upholstery, and pillows. Ethylene oxide is important to the development of automotive fluids that allow cars to run in hot and cold climates. Antifreeze, brake fluids, and automotive seating are just some of the many transportation products that are made from ethylene oxide.

Sources of Ethylene Oxide: Ethylene oxide is present in the environment and is created by various sources, including plants and cooking oils. The human body also creates ethylene oxide. Exposure to ethylene oxide varies across urban, suburban and rural environments. Ethylene Oxide emissions from industrial manufacturing and other applications are strictly regulated under federal and in some cases state and local laws.

Molecular Structure of Ethylene Oxide: Ethylene oxide is an organic compound with the formula C_2H_4O. It is a cyclic ether and the simplest epoxide: a three-membered ring consisting of one oxygen atom and two carbon atoms.

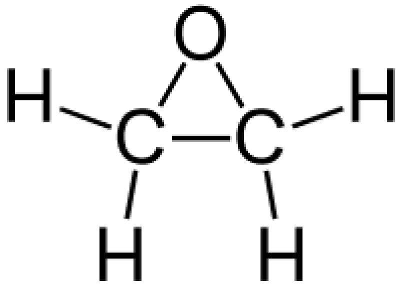


Fig 1: Molecular structure of Ethylene Oxide

CHAPTER 2: LITERATURE REVIEW

Ethylene oxide has been produced commercially by two basic routes: the ethylene chlorohydrin and direct oxidation processes. The chlorohydrin process was first introduced during World War I in Germany by Badische Anilin-und Soda-Fabrik (BASF) and others. 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. Union Carbide Corporation was the first to commercialize this process in the United States in 1925. 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, as the name implies, 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. Union Carbide Corp. was the first to commercialize an air-based direct oxidation process in 1937. The first oxygen-based system was commercialized by Shell Oil Co. in 1958.

Several companies have developed technologies for direct oxidation plants. Union Carbide Corporation and Dow Chemical use their own technologies. Shell Development, Scientific Design, and more recently, Nippon Shokubai, license ethylene oxide technology, and over 70% of present world capacity is based on their processes. Shell and Nippon Shokubai technologies are solely oxygen-based, and Scientific Design offers both air and oxygen based processes. All the ethylene oxide plants that have been built during the last 15 years were oxygen-based processes, and a number of existing ethylene oxide plants were converted from the air to the oxygen-based process during the same period. Extensive information on the early developments of the chlorohydrin and direct oxidation processes are reported. The total world production capacity of ethylene oxide in 1992 was about 106 metric tons. Most ethylene oxide is consumed by its producers in making derivatives. From Literature Review we found that there are many processes for the production of Ethylene Oxide. Here we are describing different processes for manufacturing Ethylene Oxide.

Reference:https://www.osha.gov/ethylene oxide#:~:text=Ethylene%20oxide%20(EtO)%20is%20produced,for%20medical%20equipment%20and%20supplies

We have reviewed additional research papers, and some important points from these are highlighted accordingly.

Ethylene Oxide

(SIEGFRIED REBSDAT, Winh€oring, Federal Republic of Germany

DIETER MAYER, Hoechst Aktiengesellschaft, Frankfurt, Federal Republic of Germany)

1. chlorohydrin process for manufacturing ethylene oxide involves eliminating. The hydrochloric acid from ethylene chlorohydrin.
2. The process was discovered by WURTZ in 1859 and industrial production based on this method began in 1914.
3. This process involves the reaction of ethylene with chlorine and water, leading to the formation of ethylene chlorohydrin, which is then treated to obtain ethylene oxide.

Oxidation of Ethylene to Ethylene Oxide

(Shen-Wu Wan)

1. Two commercial processes for manufacturing ethylene oxide include a two-step procedure involving ethylene chlorohydrin as an intermediate and a one-step direct oxidation of ethylene using a silver catalyst.
2. McClellan highlighted the scarcity of published data on plant design and experimental results using the direct oxidation process.
3. Twigg conducted a study on the reaction mechanism of ethylene oxidation under different conditions, while Messing indicated investigations into using oxygen instead of air.

Method for preparation of ethylene oxide by ethylene epoxidation

(Gao Shuang Zhang Yi Zhao Gongda Lv Ying Li Jun)

1. The invention relates to a method for preparation of ethylene oxide by ethylene epoxidation.
2. Utilizes a reaction-controlled phase transfer catalyst for ethylene epoxidation.
3. Incorporates an additive to improve ethylene oxide yield and selectivity.

CHAPTER 3: PROPERTIES OF ETHYLENE OXIDE

Property	**SI Units**	**Engineering Units**
Molecular Weight	44.053	44.053
Liq. Sp. Gr. 20°C/20°C (68°F/68°F)	0.875	0.875
Melting Point	160.65 K	-170.5°F
Heat of Fusion at Melting Point	117.5 kJ/kg	50.52 BTU/lb
Normal Boiling Point at 101.325 kPa (1 atm)	283.6 K	50.8°F
Heat of Vaporization	579.5 kJ/kg	249.2 BTU/lb
Heat of Formation-Ideal Gas	-1194.8 kJ/kg	-514 BTU/lb
Heat of Formation-Liquid		-129.15 BTU/lb
Standard Heat of Combustion (Liquid HHC) (HHV) (to water condensed)	-29,076 kJ/kg	-12,509 BTU/lb
Standard Heat of Combustion (Gas LHC) (LHV) (to water as vapor)	-27,649 kJ/kg	-11,895 BTU/lb
Standard Heat of Combustion (Gas HHC) (HHV) (to water condensed)	-29,647 kJ/kg	-12,755 BTU/lb
Heat of Solution in Water	-142.7 kJ/kg	-61.35 BTU/lb
Electrical Conductivity (liq)	46-06 Siemens/m	4E-08 mhos/cm
Liq Dielectric Const at 0°C (32°F)	14.5	14.5
Vapor Dielectric Const at 15°C (54.5°F)	1.01	1.01
Flash Point	<255.16 K	<O°F

Table 1: Properties of Ethylene Oxide

CHAPTER 4: DIFFERENT PROCESSES FOR PRODUCTION OF ETHYLENE OXIDE

Chlorohydrin Process: Ethylene oxide is produced from ethylene chlorohydrin by dehydrochlorination using either sodium or calcium hydroxide The by-products include calcium chloride, dichloroethane, bis(2-chloroethyl) ether, and acetaldehyde. Although the chlorohydrin process appears simpler, its capital costs are higher, largely due to material of construction considerations.

Arsenic Catalyzed Liquid Phase Process: An arsenic catalyst liquid-phase process for olefin oxides has been patented by Union Carbide. The selective epoxidation of ethylene by hydrogen peroxide in a 1,4-dioxane solvent in the presence of an arsenic catalyst is claimed. No solvent degradation is observed. Ethylene oxide is the only significant product detected. The catalyst used may be either elemental arsenic, an arsenic compound, or both.

Thallium-Catalyzed Epoxidation Process: The use of Tl(III) for olefin oxidation to yield glycols, carbonyls, or epoxides is well known. Because the epoxidation with Tl(III) is stoichiometric to produce Tl(I), reoxidation is needed. Halcon has patented processes based on such epoxidation to yield ethylene oxide. The primary benefits of such a process are claimed to be high yields of ethylene oxide, flexibility to produce either propylene oxide or ethylene oxide, and the potential of a useful by-product (acetaldehyde). Advances using organic hydroperoxides in place of oxygen for reoxidation offer considerable promise, since reaction rates are rapid and low pressures can be used.

Lummus Hypochlorite Process: A Lummus patent claims a process for propylene oxide or ethylene oxide using tert-butyl hypochlorite. The chemistry for this new process parallels the classical chlorohydrin technology with brine recycle. Advantages claimed are high ethylene yield, reduced reactor size, and lower steam requirements for the saponification step. However, disadvantages include high capital cost for a large chlorine plant, difficult and energy-intensive distillation steps, and losses of tert-butyl alcohol in the process.

Electrochemical Process: Several patents claim that ethylene oxide is produced in good yields in addition to faradic quantities of substantially pure hydrogen when water and ethylene react in an electrochemical cell to form ethylene oxide and hydrogen. The only raw materials that are utilized in the ethylene oxide formation are ethylene, water, and electrical energy. The electrolyte is regenerated in situ, ie, within the electrolytic cell. The addition of oxygen to the ethylene is activated by a catalyst such as elemental silver or its compounds at the anode or its vicinity. The common electrolytes used are water-soluble alkali metal phosphates, borates, sulfates, or chromates at 22-25 C. The process can be either batch or continuous.

Unsteady-State Direct Oxidation Process: Periodic interruption of the feeds can be used to reduce the sharp temperature gradient assoociated with the conventional oxidation of ethylene over a silver catalyst. Steady and periodic operation of a packed-bed reactor has been investigated for the production of ethylene oxide. By periodically varying the inlet feed concentration of ethylene or oxygen, or both, considerable improvements in the selectivity to ethylene oxide were claimed. The use of a fluidized bed for ethylene oxide production was reported to produce good temperature control and inhibition of side reactions using a granular silver catalyst. Several additional fluid-bed processes that claim improved product yields were patented later. However, only one process, developed by Vulcan Atlantic, was reported to have been successfully demonstrated in pilot-scale equipment. The pilot fluid-bed reactor is described as a multitubed converter that produces uniform heat transfer to a fluid circulating in the shell of the converter, and minimizes back-mixing of the fluidized catalyst. A novel circulating fluid-bed process and the associated reaction apparatus have been patented. By employing high gas velocities, the ethylene oxide productivity per unit catalyst volume is claimed to be three to four times greater than the maximum reported number for conventional fixed-bed tubular reactor.

Direct Oxidation Process: Compared to the chlorohydrin process, direct oxidation eliminates the need for large volumes of chlorine. Also, there are no chlorinated hydrocarbon by-products to be sold, processing facilities can be made simpler, and operating costs are lower (102). 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 ca 20-25% of the ethylene to carbon dioxide and water. Consequently, operating conditions must be carefully controlled to maximize selectivity. 5 To prevent further oxidation of ethylene oxide, the ethylene conversion of the commercial processes is typically between 10 and 20%. Although these reactions have been researched extensively and are the subjects of numerous patents, the precise reaction mechanism is not fully understood. The controversy has mostly centered on the nature of the oxygen species responsible for ethylene oxide formation (103). The results of various surface characterization studies indicate that there are at least three types of adsorbed oxygen species on silver: monoatomic chemisorbed oxygen, diatomic (molecular) oxygen, and subsurface oxygen. The first results from a dissociative adsorption of oxygen on a silver surface. The second is non dissociative, and is more weakly bonded. The third case arises when the temperature is higher than 420 K, at which point diffusion of atomic adsorbed oxygen from surface to subsurface region becomes appreciable.

In addition to ethylene oxide, carbon dioxide, and water, small quantities of acetaldehyde and traces of formaldehyde are also produced in the process. They generally total less than 0.2% of the ethylene oxide formed. Acetaldehyde is most likely formed by isomerization of ethylene oxide, whereas formaldehyde is most likely formed by direct oxidation of ethylene.

Unsteady-State Direct Oxidation Process:

Advantages/Disadvantages of Oxygen Based Direct Oxidation Process:

Advantages:

1)High selectivity ~75%

2)No purge reactor required

3)Requires a minimum amount of catalyst

4)Higher capacities are more economical

Disadvantages:

1)Instruments - expensive

2)Extra feedstock is required for CO_2 removal

Advantages/Disadvantages of Air Based Direct Oxidation Process:

Advantages:

1)Cheap Operating Costs

2)Low purity ethylene

3)Very safe process

Disadvantages:

1)Requires a purge reactor

2)Air purification required

3)Lowest selectivity at 70%

COMPARISON TABLE:

Here is a table consisting a comparison among the three processes for the production of Ethylene Oxide:

Method	Chlorohydrin Process	Direct Oxidation Process	Direct Epoxidation Pprocess
Reaction	1. $C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$ (Ethylene dichloride) 2. $C_2H_4Cl_2 + NaOH \rightarrow C_2H_4O$ (Ethylene oxide) + $NaCl + H_2O$	1. $C_2H_4 + O_2 \rightarrow C_2H_4O$ (Ethylene oxide)	• $C_2H_4 + O_2 \rightarrow C_2H_4O$ (Ethylene oxide)
Key Features	• Involves the intermediate formation of ethylene dichloride (chlorohydrin). • Historically widely used but declining in popularity due to environmental concerns.	• Direct oxidation of ethylene with oxygen or air. • Simplified process compared to the chlorohydrin process.	• Direct catalytic oxidation of ethylene with oxygen or air. • Eliminates intermediate formation of chlorohydrin.
Advantages	• Established industrial process. • Relatively mature technology.	• Potentially more environmentally friendly due to avoidance of chlorine-containing compounds. • Offers the potential for improved efficiency and reduced environmental impact.	• Avoids the use of chlorine-containing compounds, potentially reducing environmental impact. • Offers a simplified process compared to the chlorohydrin process.
Disadvantages	• Generation of chlorinated by-products may pose environmental concerns. • Requires additional steps for conversion from chlorohydrin to ethylene oxide.	• Requires careful control of temperature, pressure, and catalyst activity. • Formation of unwanted by-products such as carbon dioxide may reduce overall yield.	• Challenges include maintaining catalyst stability and selectivity over extended periods. • Requires further research and development to optimize efficiency and sustainability.

Table 2: Comparison Table

From the above mentioned processes and comparison, it is clear that Oxygen based Direct Oxidation Process is the more suitable for industry scale production.

CHAPTER 5: PHYSICAL AND CHEMICAL PROPERTIIES OF REACTANTS FOR THE DIRECT OXIDATION PROCESS

Name of Raw Materials: Ethene. Oxygen, Nitrogen

Properties of Ethene/Ethylene:

Ethylene appears as a colorless gas with a sweet odor and taste. It is lighter than air. It is easily ignited and a flame can easily flash back to the source of the leak. Under prolonged exposure to fire or heat the containers may rupture violently and rocket. Can cause explosion.

Ethylene, refrigerated liquid (cryogenic liquid) appears as a pressurized liquid when shipped below 50 °F. Colorless with a sweet odor and taste. Vapors arising from the boiling liquid are lighter than air. Easily ignited. Not toxic but is a simple asphyxiant. Under prolonged exposure to fire or intense heat the containers may rupture violently and rocket. Used as an anesthetic, a refrigerant, and to make other chemicals.

Physical properties:

- At room temperature and pressure, a colourless gas exists
- -169°C melting point
- -104°C is the boiling point.
- The scent is slightly pleasant
- flammable
- Non-polar molecule that is soluble in non-polar solvents hut not polar solvents such as water
- The double bond is the active site in this reaction
- Ethene, for example, is a good candidate for additional reactions

Chemical Properties:

- Addition of Chlorine:

  $CH_2=CH_2+Cl_2CH_2Cl-CH_2C1$
  1,2-dichloroethane

- Addition of Bromine:

  $CH_2=CH_2+Br_2CH_2Br-CH_2Br$
  1,2-dibromoethane

- Addition of H2O:

  $CH_2=CH_2+HOH$—>CH3-CH2-OH

The two carbon atoms form a sigma bond in the molecule by overlapping two sp2orbitals. Each carbon atom forms two covalent bonds with hydrogen by s-sp2overlap, all with 120° angles. 2p-2p overlap forms the pi bond between carbon atoms perpendicular to the molecular plane Ethylene is used in two ways: as a monomer from which longer carbon chains can be built, and as a starting material for other two-carbon compounds.

Properties of Oxygen:

Oxygen comprises 21 percent of the gasses present in the earth's atmosphere and has very distinct characteristics. Like any other element there are various properties of oxygen.

The physical properties of oxygen are as follows:

Oxygen is a colorless gas.

It is an odorless gas.

Oxygen does not have any taste.

Oxygen has a higher density than air.

Oxygen is a very poor conductor of heat and electricity.

Oxygen is soluble in some liquids such as water, alcohol, etc. (solutes slightly)

The chemical properties of oxygen are as follows:

Oxygen does not burn itself but fire needs oxygen to keep burning Le, it supports combustion.

Oxygen can be in multiple types of compounds. The compounds include iron ore, water, carbon-di- oxide, etc.

When it unites with other substances, it is known as the oxidation process.

Oxygen is a very strong oxidizing agent.

Reactivity-Oxygen can be produced by the process of action of UV (ultraviolet) radiation on oxygen in the stratosphere (a specific layer of the earth's atmosphere) and by the electric discharge in oxygen as well.

Oxygen has its own distinct physical and chemical properties and thus, according to those characteristics, it is used accordingly in different industries and purposes. Oxygen is used in medical applications, commercial, and industrial practices.

Properties of Nitrogen:

Physical properties of Nitrogen:

Nitrogen is a colorless, odorless, and tasteless gas.

It is slightly lighter than air.

It is slightly soluble in water.

It is a non-poisonous gas but animals die due to suffocation of nitrogen.

Chemical properties of Nitrogen:

It is non-combustible gas neither does it support burning.

It is chemically inert under ordinary conditions.

Nitrogen reacts with certain metals to form metal nitrides. Example: Nitrogen reacts with

Calcium to form Calcium nitride.

Nitrogen combines with oxygen to form oxides of nitrogen.

The chemical properties of nitrogen in chemistry and the various other concepts related to Nitrogen are discussed in the aforementioned module. Nitrogen contributes vastly to making up the vast bulk of biological material.

CHAPTER 6: PROPERTIES OF PRODUCTS FORMED IN THE OXYGEN BASED DIRECT OXIDATION METHOD: ETHYLENE OXIDE, CARBON DIOXIDE, WATER

Properties of Ethylene Oxide:

Physical properties of EO: Ethylene oxide appears as a clear colorless gas with an ethereal odor with a flash point below 0 °F. Liquid less dense than water. Vapors heavier than air. May polymerize exothermically if heated or contaminated. If the polymerization takes place inside a container, the container may rupture violently. Vapors very toxic. Vapors irritate the eyes, skin, and respiratory system. Prolonged skin contact may result in delayed burns. Used to make other chemicals, as a fumigant and industrial sterilant.

Chemical Properties of EO: Ethylene oxide readily reacts with diverse compounds with opening of the ring. Its typical reactions are with nucleophiles which proceed via the SN2 mechanism both in acidic (weak nucleophiles: water, alcohols) and alkaline media (strong nucleophiles: OH-, RO, NH3 RNH2 RR'NH, etc.)

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.

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

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

Ethylene oxide readily reacts with aqueous solutions of hydrochloric, hydrobromic and hydroiodic acids to form halohydrins.

Interaction of ethylene oxide with organomagnesium compounds, which are Grignard reagents, can be regarded as nucleophilic substitution influenced by carbanion organometallic compounds. Addition of hydrogen cyanide Ethylene oxide easily reacts with hydrogen cyanide forming ethylene cyanohydrin.

When reacting with the hydrogen sulfide, ethylene oxide forms 2-mercaptocthanol and thiodiglycol, and with alkylmercaptans it produces 2-alkyl mercaptoctanol.

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

In the presence of alkoxides, reactions of ethylene oxide with compounds containing active methylene group leads to the formation of butyrolactones etc.

Properties of Carbon Dioxide:

Physical Properties of Carbon Dioxide:

CO_2 naturally exists in the gaseous form. Its molar mass is 44gmol-1. It has a melting point of -55.60C. i.e., it exists in the solid form below this temperature. In the solid form, it is known as dry ice, and it should not be handled with utmost care as it can cause damage to the skin. It is a linear and covalent molecule that is slightly soluble in water. As the temperature increases, the solubility in water decreases.

In gaseous form, it is colorless and odorless. It has a sour taste. It is a dense gas, with a density of 1.977gmL-I. Due to this, it is heavier than air and can displace oxygen. It is acidic in nature and forms a weak acid called carbonic acid when dissolved in water. It can turn blue litmus paper red.

The gas is non-flammable, making it especially useful for applications in fire extinguishers. The presence of oxygen is crucial for combustion to take place. Carbon dioxide in fire extinguishers cuts the supply of oxygen from the fuel source due to which fire is doused.

$0_2+CH_4 \rightarrow CO_2+ H_20$ (combustion reaction)

In high concentrations, it is toxic to humans and has a pungent odor. When exposed to pure carbon dioxide, the person collapses and eventually dies when they are unable to get oxygen. At low concentrations, however, it is relatively non-toxic and odorless.

Chemical Properties of Carbon Dioxide:

The chemical properties of carbon dioxide are very much influenced by the acidic behaviour of the gas. For example, it reacts with water to form carbonic acid, which is a weak acid. It dissociated partially into hydronium and carbonate ions.

$CO_2+H_2O \rightarrow H_2CO_3$

$H_2CO_3 \rightleftharpoons H++HCO_3-$

$HCO_3 \rightleftharpoons H++ CO_2-$

Since it is acidic, it reacts with basic compounds as per the neutralisation reaction, giving salt and water.
Reaction of carbon dioxide with sodium hydroxide:

CO2+2NaOH→ Na2CO3+H2O

In the presence of excess carbon dioxide, the following reaction occurs,

Na2CO3+H2O+CO2→2NaHCO3

$NaHCO_3$, or sodium bicarbonate, is an alkali. It is a salt of a weak acid (carbon dioxide) and a strong base (NaOH). $NaHCO_3$ has several uses. It is used in the kitchen as it makes dough fluffy and raises it.

$2NaHCO_3+H+ Na_2CO_3+CO_2+H_2O$

In the presence of acid (which is present in food) and heat, baking soda gives the above reaction in which CO_2 is evolved. This evolved carbon dioxide makes the dough fluffy.
Reaction with metals Chemical properties of carbon dioxide involve reaction with metals to form metal oxides, which are basic in nature.

$CO2+2Mg \rightarrow 2MgO+C$

Reaction with metal oxides: CO2 reacts with group 1 and 2 metal oxides to form metal carbonates via exothermic reactions.

$CO_2 +CaO \rightarrow CaCO_3$

Properties of Water:

Physical Properties of Water:

The molecules in water have hydrogen bonding between them. The boiling and melting point of water are 100 and 10° C respectively.
The three states water can have are solids, liquids, and gas.
Water has a polar nature because of which it can dissolve almost every substance and is hence called the universal solvent.
In the solid state, water possesses a crystalline structure which is a cage-like structure in the form of 3-D.
The crystalline structure of water has many voids due to which the density of ice is less than water and hence can float on water.
The density of water is known to be as 0.99 g/ml. at 4°C.

Chemical properties of water:

Water reacts with a lot of substances to form different compounds. Some significant reactions are as follows:
Amphoteric nature:
Water can act as both acid and base, which means that it is amphoteric in nature.
Redox reactions:
Electropositive elements reduce water so hydrogen molecule. Thus, water is a great source of hydrogen. Let us see an example in this case:
During the process of photosynthesis, water is oxidized to 02. As water can be oxidized and reduced, it is very useful in redox reactions.
Hydrolysis reaction Water has a very strong hydrating tendency due to its dielectric constant. It dissolves many ionic compounds. Some covalent and ionic compounds can be hydrolyzed in water.

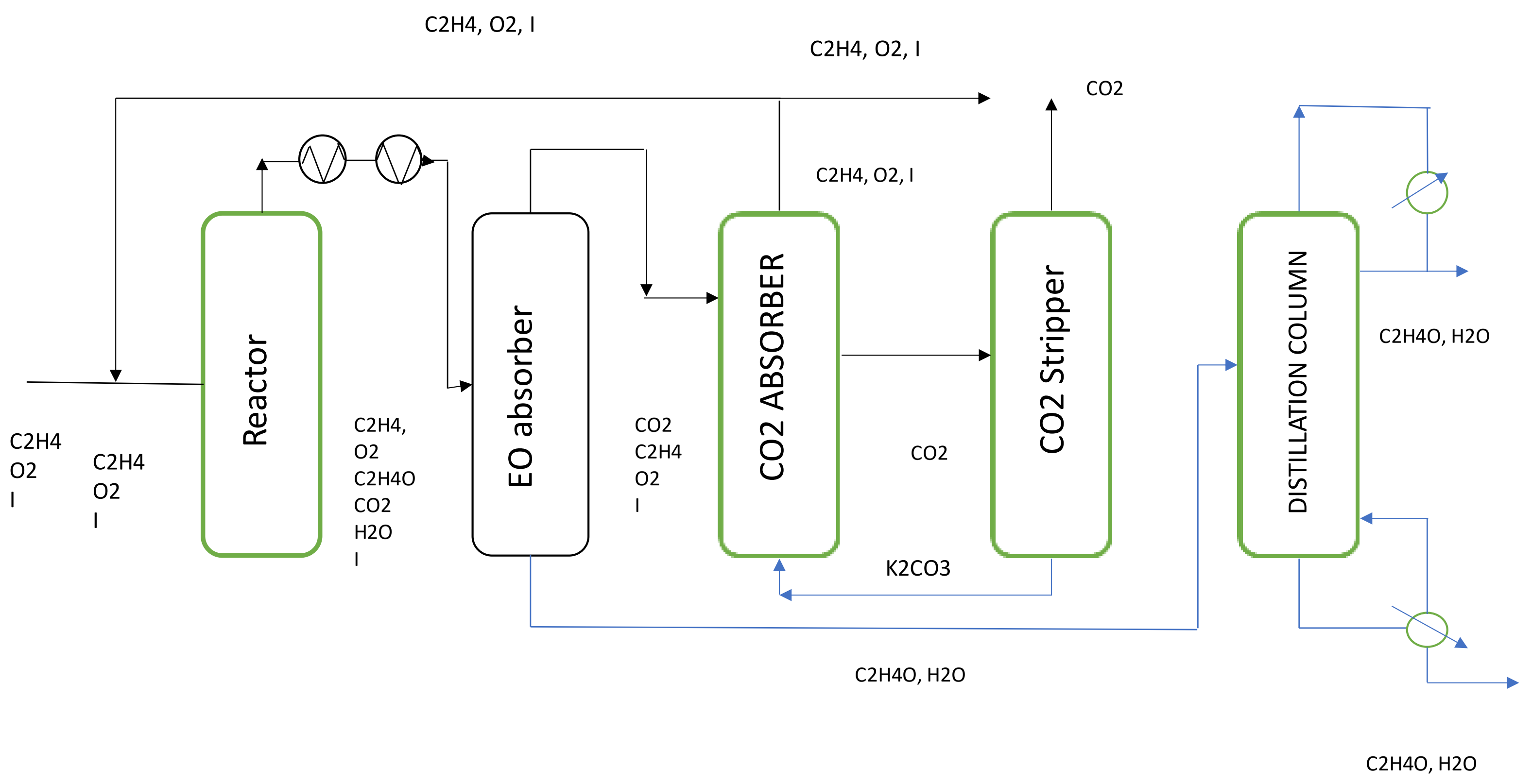


Figure 2: Flowsheet for Oxygen based Direct Oxidation Process

CHAPTER 7: MATERIAL BALANCE

REACTOR:

Basis: 1000 kmol/ hr

The two reactions taking place in oxygen based direct oxidation process are given below:

All ethylene oxide direct oxidation plants are based on original process chemistry discovered by Lefort in 1931, the main reaction is –

$C_2H_4 + \frac{1}{2} O_2 \rightarrow C_2H_4O$

Only significant byproducts are carbon dioxide and water which are formed by complete combustion of ethylene.

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

Molecular weights of the compounds:

Compounds	Molecular weights
Ethene/ Ethylene	28
Oxygen	32
Ethylene oxide	44
Carbon dioxide	44
Water	18
Nitrogen	28

Table 3: Molecular weights of compounds

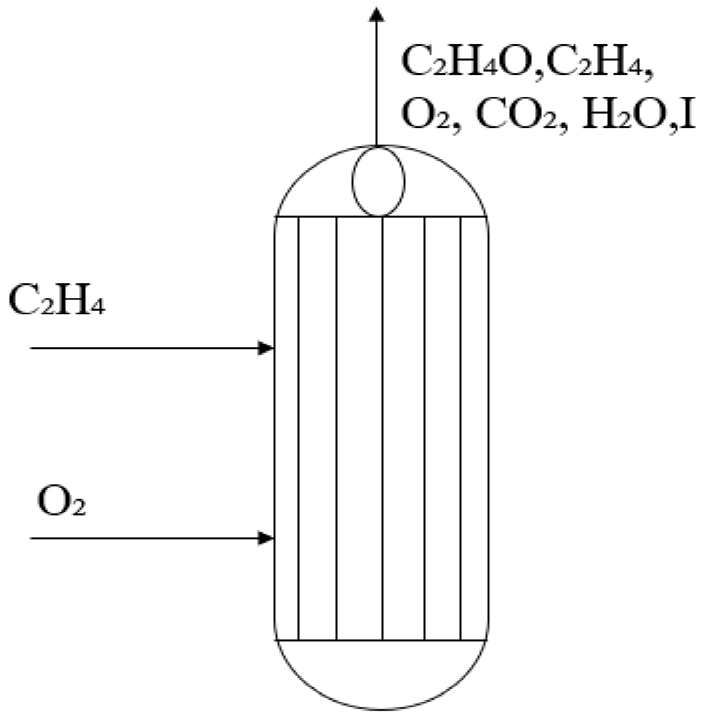


Figure 3: Reactor

Material balance for reactor:

$C_2H_4 + \frac{1}{2}$ O2 ➔ C_2H_4O (Main reaction)

$C_2H_4 + 3O_2$ ➔ $2CO_2 + 2H_2O$ (Side reaction)

Assumptions:

- Commercial grade ethylene (99.9%) pure C_2H_4; where 0.01% are impurity.
- Air: Ethylene ratio = 9:1
- the conversion of ethylene in the main reaction is 1/3rd of the total feed where rest 2/3rd converts into byproducts and 1/3rd of the total C_2H_4 remained as it is as C_2H_4 (unreacted).

C_2H_4 reacted = $99.9 * \frac{33.33}{100}$ = 33.3 kmol/hr

O_2 reacted = 16.65 kmol/hr

C_2H_4O produced = 33.3 kmol/hr

From side reaction,

$C_2H_4 + 3O_2$ ➔ $2CO_2 + 2H_2O$

For 1 mole of CO_2

$99.9 * \frac{33.33}{100}$ = 33.3 kmol/hr

For 2 moles of CO_2 = 66.6 kmol/hr

For 2 moles of H2O = 66.60 kmol/hr

O_2 consumed in the main reaction = 16.65 kmol/hr

O_2 consumed in the side reaction = $33.3 * 3$ = 99.9 kmol/hr

Therefore, total oxygen left = 189 – (16.65 + 99.9)

= 72.45 kmol/hr

C_2H_4 unreacted = $\frac{1}{3} * 99.9$ = 33.3 kmol/hr

	Feed		Output	
Compound	kmol/hr	kg/hr	kmol/hr	kg/hr
C_2H_4	99.9	2797.2	33.3	932.4
O_2	189	6048	72.45	2318.4
C_2H_4O	-	-	33.3	1465.2
CO_2	-	-	66.6	2930.4
H_2O	-	-	66.6	1198.8
N_2	711	19908	711	19908
Total		28753.26		28753.2

Table 4: Material Balance for Reactor

HEAT EXCHANGER 1:

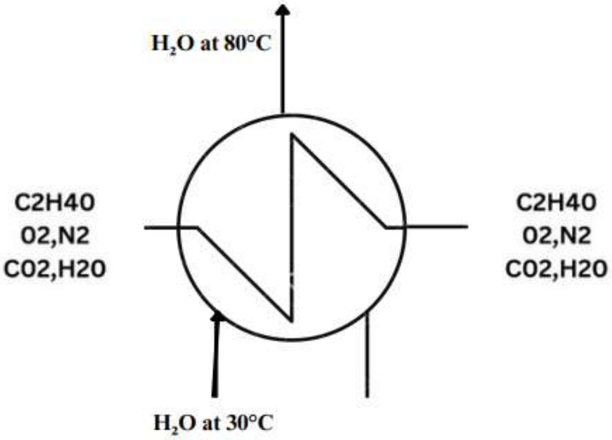


Figure 4: Heat Exchanger 1

The products formed are now passed through a heat exchanger to cooled from 250 to 100^{O}C. So only the temperature change has occurred.

	Input		Output	
Compound	kmol/hr	kg/hr	kmol/hr	kg/hr
C_2H_4	99.9	2797.2	33.3	932.4
O_2	189	6048	72.45	2318.4
C_2H_4O	-	-	33.30	1465.2
CO_2	-	-	66.60	2930.4
H_2O	-	-	66.60	1198.8
N_2	711	19908	711	19908
Total		28753.26		28753.26

Table 5: Material Balance for Heat Exchanger 1

HEAT EXCHANGER 2:

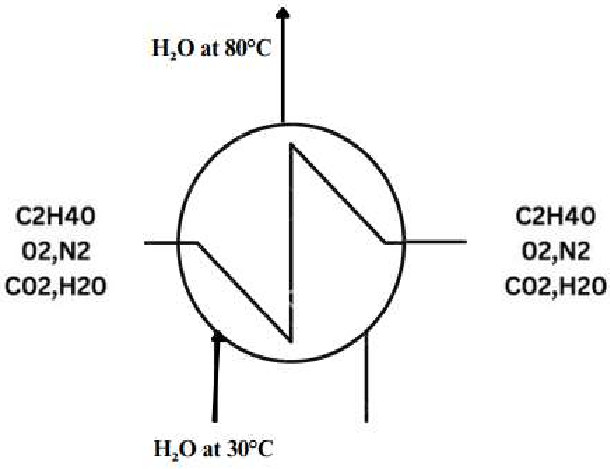


Figure 5: Heat Exchanger 2

Now the steam is passed through another heat exchanger to be cooled from 100 to 8^{O}C. Again, only temperature change has occurred.

Output of the first heat exchanger is the input to the second heat exchanger.

	Input		Output	
Compound	kmol/hr	kg/hr	kmol/hr	kg/hr
C_2H_4	99.9	2797.2	33.3	932.4
O_2	189	6048	72.45	2318.4
C_2H_4O	-	-	33.30	1465.2
CO_2	-	-	66.60	2930.4
H_2O	-	-	66.60	1198.8
N_2	711	19908	711	19908
Total		28753.26		28753.26

Table 6: Material Balance for Heat Exchanger 2

EO ABSORBER:

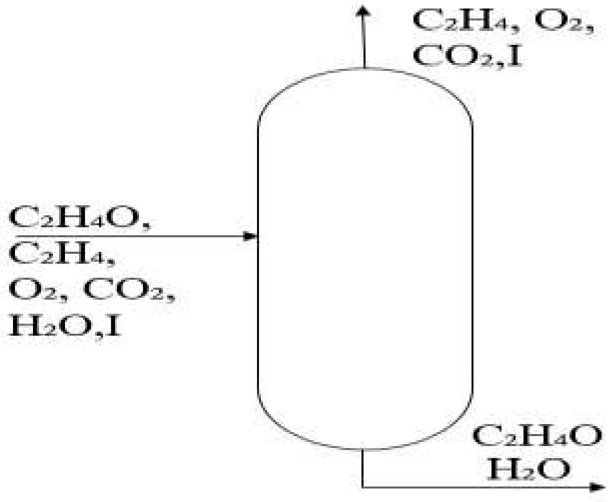


Figure 6: EO Absorber

	Input		Output		
Compound	kmol/hr	kg/hr		kmol/hr	kg/hr
C_2H_4	33.3	932.4	Top	33.3	932.4
O_2	72.45	2318.4		72.45	2318.4
N_2	711	19908		711	19908
CO_2	66.6	2930.4		66.6	2930.4
H_2O	66.6	1198.8	Bottom	66.6	1198.8
C_2H_4O	33.3	1465.2		33.3	1465.2
Total		28753.2			28753.2

Table 7: Material Balance for EO Absorber

CO_2 ABSORBER:

Assumptions:

- 100% CO_2 is absorbed.

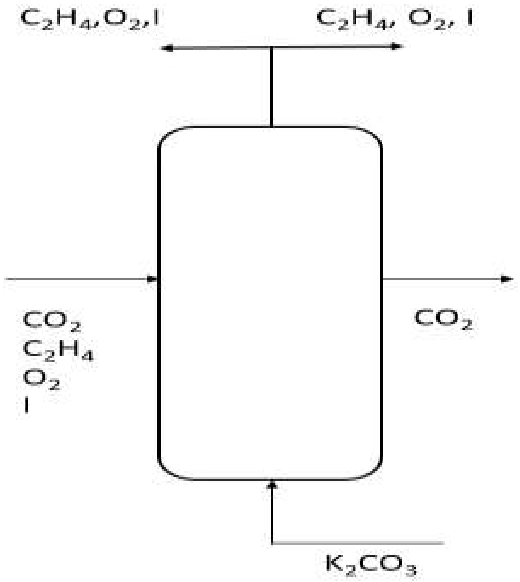


Figure 7: CO_2 Absorber

	Input		Output		
Compound	kmol/hr	kg/hr		kmol/hr	kg/hr
C_2H_4	33.3	932.4	Unabsorbed	33.3	932.4
O_2	72.45	2318.4		72.45	2318.4
N_2	711	19908		711	19908
CO_2	66.6	2930.4	Absorbed gas	66.6	2930.4
Total		26087.6			26087.6

Table 8: Material Balance for CO_2 Absorber

CO_2 STRIPPER:

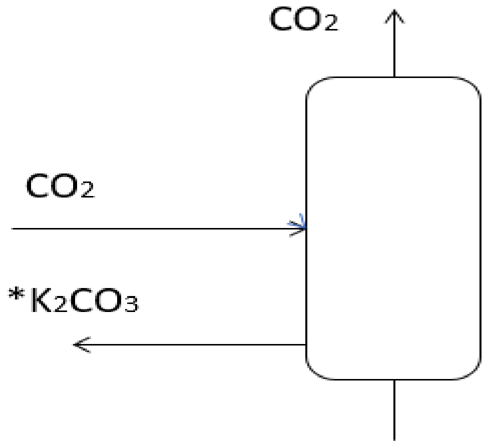
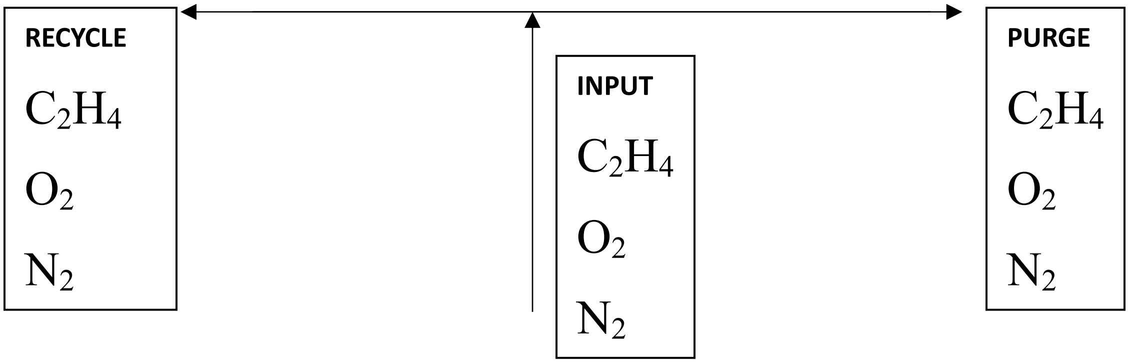


Figure 8: CO_2 Absorber

*K_2CO_3 is used for absorbing medium

	Input		Output		
Compound	kmol/hr	kg/hr		kmol/hr	kg/hr
CO_2	66.6	2930.4	Absorbed gas	66.6	2930.4
Total		2930.4			2930.4

RECYCLE POINT



	Input		Output			
			Recycle		Purge	
Compound	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr
C_2H_4	33.3	932.4	31.635	932.4	1.665	46.62
O_2	72.45	2318.4	68.8275	2318.4	3.6225	115.92
N_2	711	19908	675.45	19908	35.55	995.4
Subtotal				22000.86		1157.94
Total	23158.8		23158.8			

Table 9: Material Balance for CO_2 Stripper

Assuming, Recycle ➔95%

Purge➔5%

Input + Recycle ➔ Feed

Input = 28753.2 – 22000.86 = 6752.34 kg/hr

Recycle ratio = $\frac{Recycle}{Input} = \frac{22000.86}{6752.34}$ = 3.2583:1

DISTILLATION COLUMN:

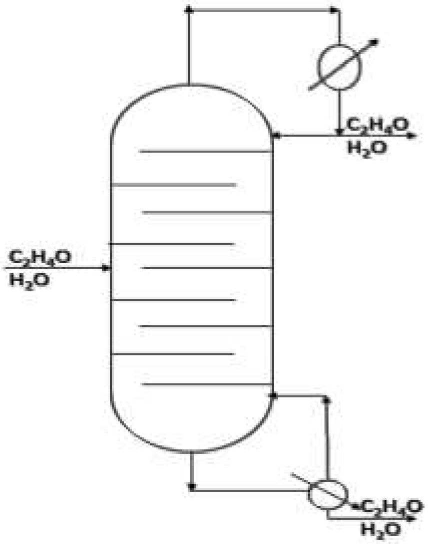


Figure 9: Distillation Column

	Input		Output		
Compound	kmol/hr	kg/hr	Compound	kmol/hr	kg/hr
C_2H_4	33.30	1465.2	Top product		
			C_2H_4O (75%)	24.975	1098.9
			H_2O (25%)	16.65	299.7
H_2O	66.60	1198.8	Bottom product		
			C_2H_4O (25%)	8.325	366.3
			H_2O (75%)	49.95	899.1
Total		2664			2664

Table 10: Material Balance for Distillation Column

CHAPTER 8: MODIFIED MATERIAL BALANCE

Capacity of the plant producing ethylene oxide = 45000 tonne per 330 working days per year

Capacity of ethylene oxide plant = 5681.81 kg/hr

Ethylene produced = 1392 kg/hr

Scale up factor = 4.081

Reactor:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	2797.2	11415.3732	407.6919
O_2	6048	24681.888	771.309
N2	19908	81244.548	2901.591

Output

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
C_2H_4O	1465.2	5979.4812	135.8973
CO_2	2930.4	11958.9624	271.7946
H_2O	1198.8	4892.3028	271.7946
N_2	19908	81244.548	2901.591

Table 11: Modified Material Balance for Reactor

<u>EO Absorber</u>:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
C_2H_4O	1465.2	5979.4812	135.8973
CO_2	2930.4	11958.9624	271.7946
H_2O	1198.8	4892.3028	271.7946
Inert	19908	81244.548	2901.591

Output

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
Top			
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
CO_2	2930.4	11958.9624	271.7946
Inert	19908	81244.548	2901.591
Bottom			
C_2H_4O	1465.2	5979.4812	135.8973
H_2O	1198.8	4892.3028	271.7946

Table 12: Modified Material Balance for EO Absorber

CO2 Absorber:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
CO_2	2930.4	11958.9624	271.7946
Inert	19908	81244.548	2901.591

Output

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
CO_2	2930.4	11958.9624	271.7946
Inert	19908	81244.548	2901.591

Table 13: Modified Material Balance for CO_2 Absorber

CO_2 Stripper:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
CO_2	2930.4	11958.9624	271.7946

Output

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
CO_2	2930.4	11958.9624	271.7946

Table 14: Modified Material Balance for CO_2 Stripper

<u>Recycle</u>:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	932.4	3805.1244	135.8973
O_2	2318.4	9461.3904	295.668
Inert	19908	81244.548	2901.591

Output

Component	Recycle			Purge		
	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4	888.38	3627.11	129.539	46.62	190.256	6.7748
O_2	2202.48	8988.3208	280.88	115.92	473.069	14.78
Inert	18912.6	77182.3206	2756.5	995.4	4062.2274	145.0795

Table 15: Modified Material Balance for Recycle

<u>Distillation Column</u>:

Input

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
C_2H_4O	1465.2	5979.4812	135.8973
H_2O	1198.8	4892.3028	271.7946

Output

Component	Kg/hr	Modified (Kg/hr)	Modified (Kmol/hr)
Top			
C_2H_4O	932.4	3805.1244	135.8973
H_2O	2318.4	9461.3904	295.668
Bottom			
C_2H_4O	1465.2	5979.4812	135.8973
H_2O	1198.8	4892.3028	271.7946

Table 16: Modified Material Balance for Distillation column

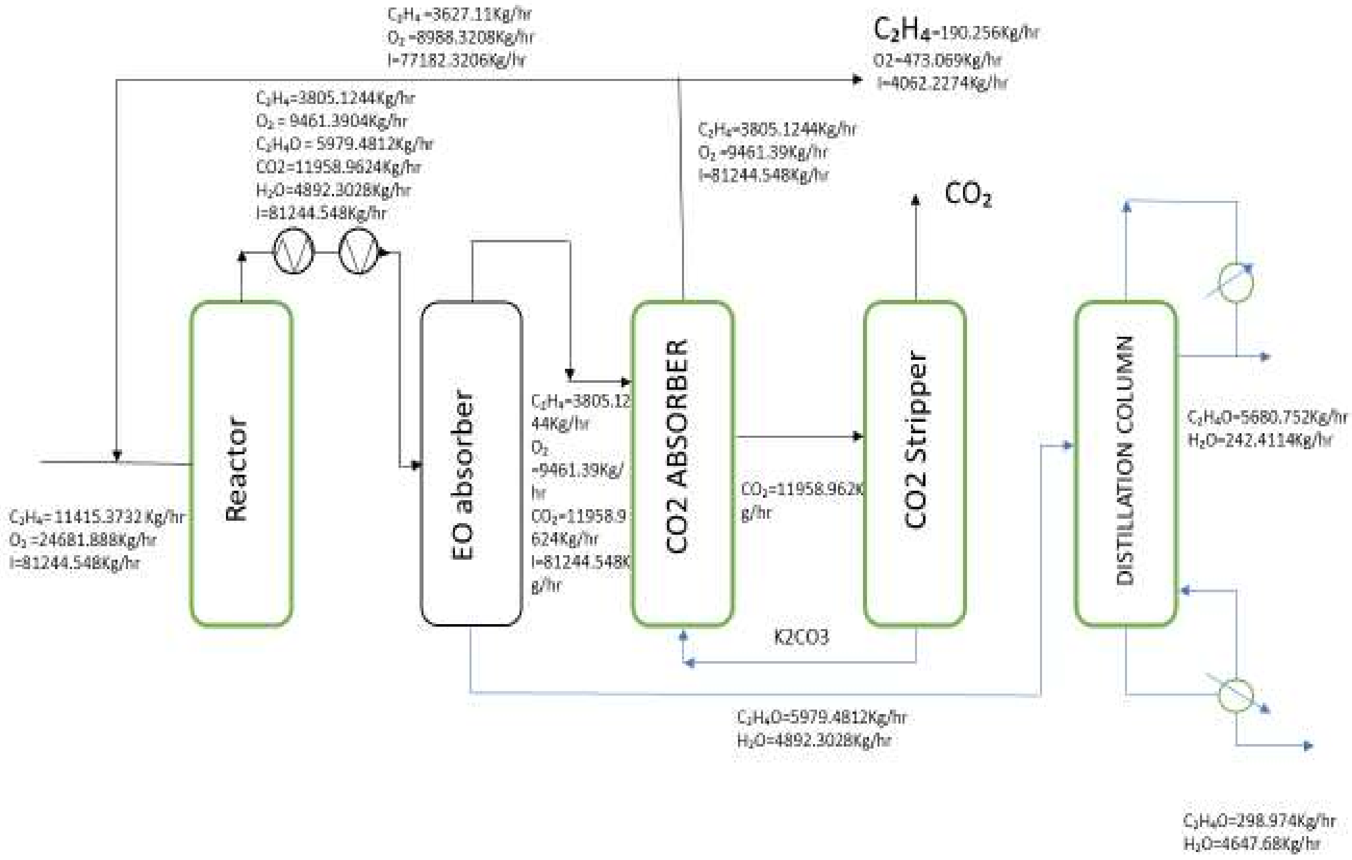
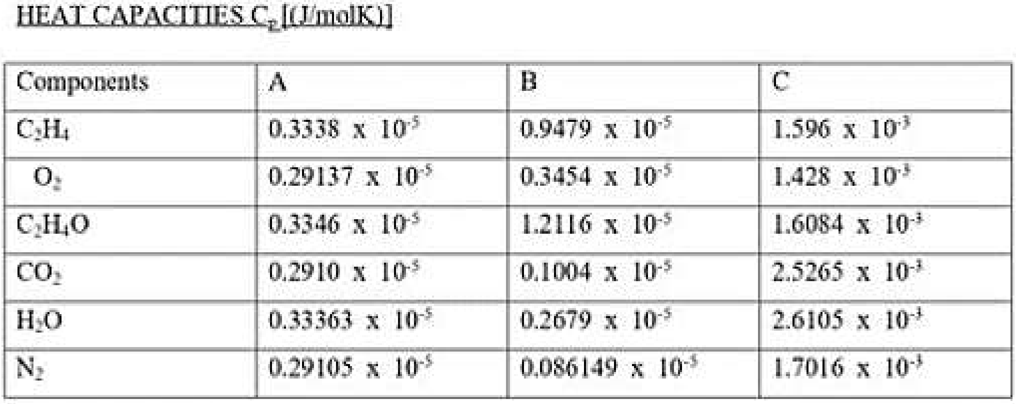


Fig: Process Flow diagram

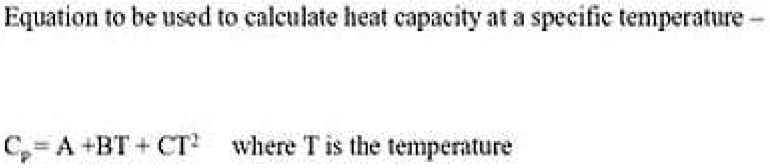
CHAPTER 9: ENERGY BALANCE



HEAT CAPACITIES C_p [(J/molK)]

Components	A	B	C
C_2H_4	0.3338×10^{-5}	0.9479×10^{-5}	1.596×10^{-3}
O_2	0.29137×10^{-5}	0.3454×10^{-5}	1.428×10^{-3}
C_2H_4O	0.3346×10^{-5}	1.2116×10^{-5}	1.6084×10^{-3}
CO_2	0.2910×10^{-5}	0.1004×10^{-5}	2.5265×10^{-3}
H_2O	0.33363×10^{-5}	0.2679×10^{-5}	2.6105×10^{-3}
N_2	0.29105×10^{-5}	0.086149×10^{-5}	1.7016×10^{-3}

Table 17: Heat Capacities



Equation to be used to calculate heat capacity at a specific temperature –

$C_p = A + BT + CT^2$ where T is the temperature

Basis:

1 hour of operation

The following assumptions are taken while calculating energy balance

1. There is no energy loss either through conduction, convection, radiation and all piping's, equipment, etc.
2. There is no pressure loss in the piping's and equipment's.
3. There is no accumulation of heat.
4. The enthalpies of all the substances are calculated taking 25°C as the datum temperature.
5. The stem used is medium pressure steam at 160Kgf/cm² which enters at 619.3K The values of Cp are calculated as-
   $Cp = a + bT + cT^2$

Energy balance for the reactor:

Products from the reactor

INPUT	Kmol/hr	OUTPUT	Kmol/hr
$C2H_4$	407.6919	C_2H_4	135.8973
O_2	771.309	O_2	295.668
I	2901.591	C_2H_4O	135.8973
		CO_2	271.7946
		H_2O	271.7946
		I	2901.591

Table 18: Products from the Reactor

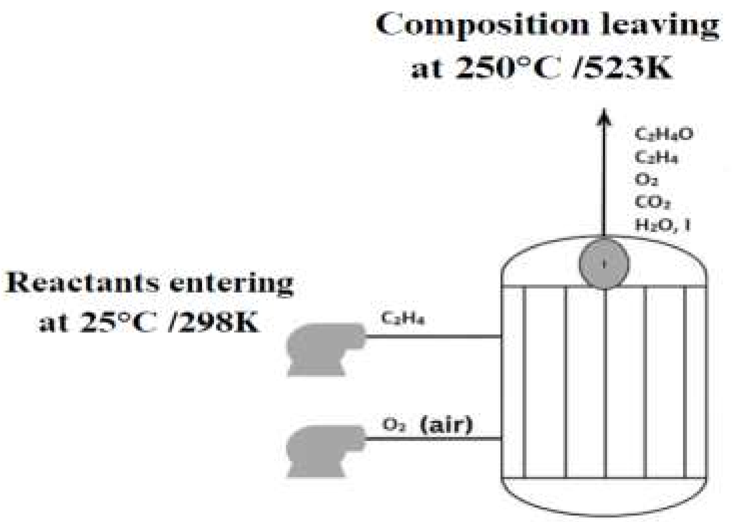


Figure: 11: Reactor

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

For 100% conversion, the enthalpies are,

Main reaction

$C_2H_4 + \frac{1}{2}O \rightarrow C2H_4O \quad \Delta H_{25} = - 106.39KJ / mol$

Side reaction

$C_2H4 + 3O_2 \rightarrow 2CO_2 + 2\ H_2O \quad \Delta H_{25} = - 1321.7KJ / mol$

Energy balance equation for the reactor

$(m\cdot Cp\cdot \Delta T)$ reactants+ΔH_{g+Q}(heat removed by exothermic reaction)= $(m\cdot Cp\cdot \Delta T)$ product

Consider feed to entering at 25°C (T_{ref} =25°C) and the reaction is occuring at 250°C

Standard Enthalpy for each conversion,

$\Delta H_{25(1)}$= - 106.39 × 1/3 = - 35.4633KJ / mol

$\Delta H_{25(2)}$= - 132.7 × 2/3 = - 881.1333KJ / mol

Heat of rxn at 25°C (25°C = 298K and 250°C =523°C)

$$\Delta H^* =(m \int_{250}^{25} Cp\, dT)_{C2H4} + (m \int_{250}^{25} Cp\, dT)_{O2}$$

=-25288256.16 - 42806220.06

=-68094476.22J/mol

=-68094.4762 KJ/mol

Again,

$$\Delta H^{**}=(m \int_{25}^{250} Cp\, dT)_{C2H4O} +(m \int_{25}^{250} Cp\, dT)_{H2O} +(m \int_{25}^{250} Cp\, dT)_{CO2}$$

=8494866.574 + 27574862.84 + 26684357.12

=62754086 J/mol

=62754.086 KJ/mol

Hence, heat of reaction at 250 °C

$\Delta H^{/}= \Delta H + \Delta H^* + H^{**}$

= - 916.5966 – 68094.4762 + 62754.086

= - 6256.9863 KJ/mol

Table: Energy Balance over the reactor

Input	KJ/mol	Output	KJ/mol
Feed	916.5966	Feed	6256.9863
Generation (Exothermic)	5340.3897	Consumption (Exothermic)	
Total	6256.9863	Total	6256.9863

Table 19: Energy Balance for Reactor

Energy balance for the heat exchanger 1:

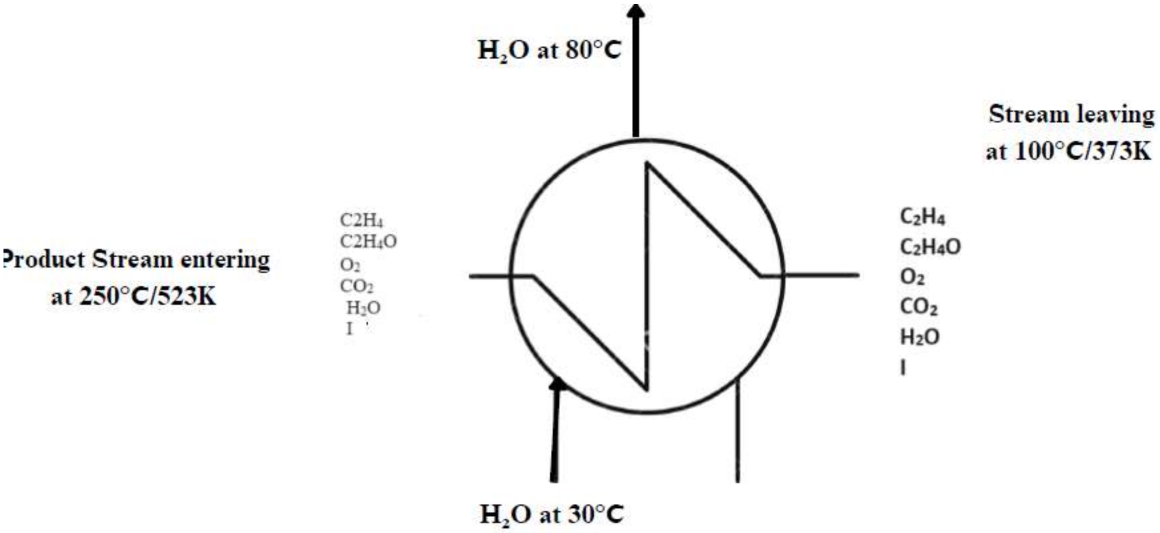


Figure 12: Heat Exchanger 1

In the cooler, product vapours are cooled from 250°C to 100°C. The energy removed is supplied to the recycle stream. The C_p, values are calculated at the temperature of 100°C.

Input to the heat exchanger = - 6256.9863 KJ/mol

Enthalpy of inlet cold water at 30°C

At liquid phase the C_p value of water is 75.9 KJ/mol

$\Delta H = (m \int_{25}^{30} Cp\, dT) = 377m$

Enthalpy of product at 100°C

$\Delta H = (m \int_{25}^{100} Cp\, dT)_{product}$

$= (m \int_{298}^{373} Cp\, dT)_{C2H4O} + (m \int_{298}^{373} Cp\, dT)_{H2O} + (m \int_{298}^{373} Cp\, dT)_{CO2}$

= 177345.9765+ 6014739.715+ 4823265.026

= 1368820.064 J/mol

= 1368.820 KJ/mol

Enthalpy of outlet water at 80°C

$\Delta H = (m \int_{25}^{80} Cp\, dT)$

= 4197m

Now,

Heat in =Heat out

- ⇨ 6256980.3 + 377m = 1368820 + 4147m
- ⇨ 3770m = 64571146.25
- ⇨ m = 17127.625 Kmol/hr
- ⇨ m = 308297.25 kg/hr (i.e Mass of water used)

Table: Energy Balance over the heat exchanger 1:

Input	KJ/mol	Output	KJ/mol
Reaction product	6256.98	Cooled Rxn product	1368.82
Cooling water	66996.4821	Cooling water	71884.6427
Total	73253.4621	Total	73253.4621

Energy balance for the heat exchanger 2:

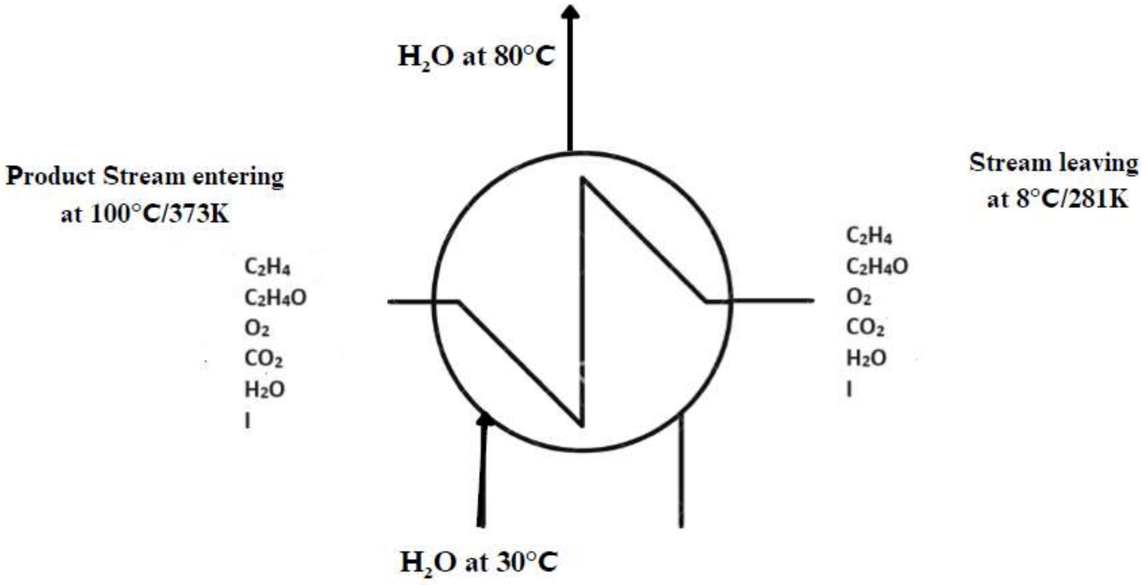


Figure 13: Heat Exchanger 2

In the cooler, product vapours are cooled from 100°C to 8°C. The energy removed is supplied to the recycle stream The C_p values are calculated at the temperature of 8°C.

Input to the heat exchanger =1368.82 KJ/mol

Enthalpy of inlet cold water at 30°C

$\Delta H = (m \int_{25}^{30} Cp\ dT) = 377m$

Enthalpy of product at 8°C

$\Delta H = (m \int_{25}^{8} Cp\ dT)_{Product}$

$= (m \int_{25}^{8} Cp\ dT)_{C2H4O} + (m \int_{25}^{8} Cp\ dT)_{H2O} + (m \int_{25}^{8} Cp\ dT)_{CO2}$

$= -31152.0778 - 101119.9579 - 97854.2098$

$= 230126.1098$ mol/hr

$= 230.126$ KJ/mol

Enthalpy of outlet cold water at 80°C

$\Delta H = (m \int_{25}^{80} Cp\, dT) = 4147m$

Now,

Heat in = Heat out

1368.82 +377m = -230.126+4147m

m = 424.1 mol/hr (i.e. mass of water used)

Table: Energy Balance over the heat exchanger 2:

Input	KJ/mol	Output	KJ/mol
Cooled Rxn product	1 368.82	Cooled Rxn product	-230.126
Cooling water	159.88	Cooling water	1758.7427
Total	1528.70	Total	1528.70

Table 21: Energy Balance for Heat Exchanger 2

Energy balance for Ethylene Oxide Absorber:

Here the feed is entering at 8°C is separated Ethylene Oxide and water from the input components. Further oxide and water are sent to the refining still.

Product Stream entering at 8°C/281K

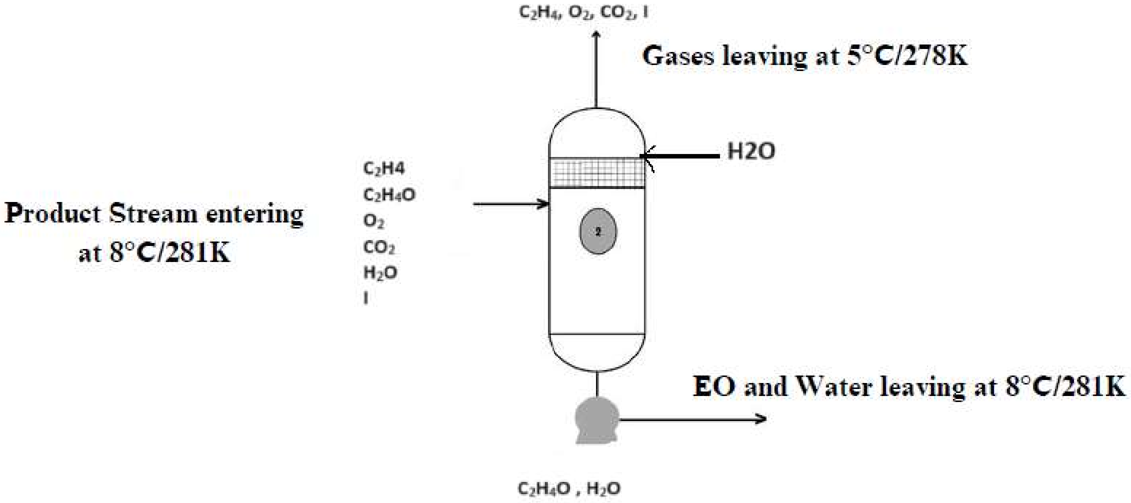


Figure 14: Ethylene Oxide Absorber

Enthalpy of Product Inlet at 8°C

ΔH =-230.126 KJ/mol

Enthalpy of Ethylene, Oxygen and Carbon Dioxide at 5°C

$\Delta H = (m \int_{298}^{278} Cp\, dT)_{C2H4} + (m \int_{298}^{278} Cp\, dT)_{O2} + (m \int_{298}^{278} Cp\, dT)_{CO2}$

$= -569803.0557 - 200689.5662 - 66225.3982$

$= -836718.02$ J/mol

$= -836.7180$ KJ/mol

Enthalpy of Ethylene Oxide and water at Bottom product

$\Delta H = (m \int_{298}^{281} Cp\, dT)_{C2H4O} + (m \int_{298}^{281} Cp\, dT)_{H2O}$

$= -311520.7887 - 295071.4838$

$= -606592.2725$ J/mol

= - 606.5922 KJ/mol

Table: Energy Balance over the Ethylene Oxide Absorber:

Input	KJ/mol	Output	KJ/mol
Cooled Rxn product	-230.126	Ethylene + Water	606.592
		Ethylene, Oxygen, Carbon Dioxide	-836.718
Total	-230.126	Total	-230.126

Table 22: Energy Balance for EO Absorber

Energy Balance for the Refining Still:

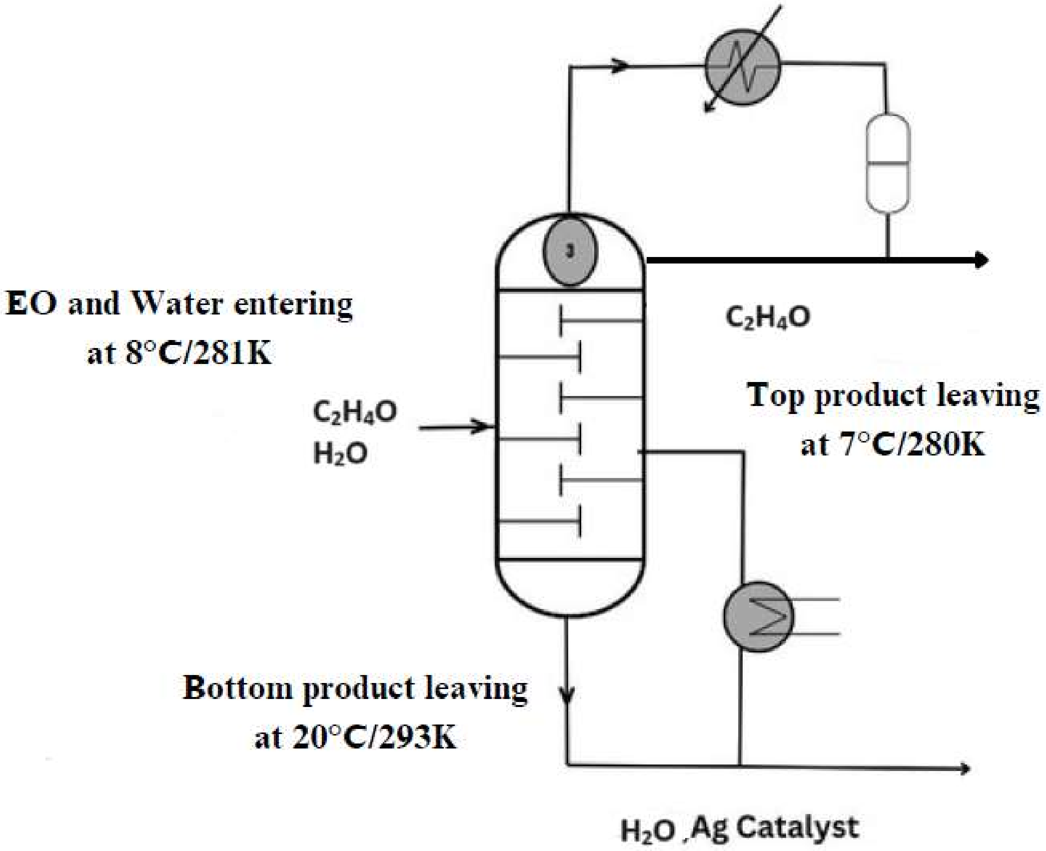


Figure 15: Refining Still

Enthalpy of the ethylene oxide and water stream at 8°C, $\Delta H_f = 606.592$ KJ/mol

Enthalpy of Distillate at 7°C (Top) Ethylene Oxide ($C_p = 0.3346\times10^{-5} + 1.2116\times10^{-5}\,T + 1.6084\times10^{-3}T^2$)

$\Delta H_D = (m \int_{298}^{280} C_p\, dT)_{C2H4O}$

$=129.108\times(-2418.8779)$ J/mol

$=-312.296$ KJ/mol

Enthalpy of bottom at 20°C ($C_p = 0.33363\times10^{-5} + 0.02679\times10^{-5}\,T + 2.6105\times10^{-3}T^2$)

$\Delta H_W = (m \int_{298}^{293} C_p\, dT)_{C2H4O}$

$=258.2048 \times 1139.7785$

$=-294.296$ KJ/mol

For condenser duty at 7°C/280K

At liquid phase,

Ethylene Oxide, $\Delta H_L = mC_pT$

$= \{129.108[0.3346 + 1.2116(280) + 160.84(280)^2]\} \times 10^{-5}$

= 16.280KJ / mol

At vapor phase

Ethylene Oxide, $\Delta H_V = \{129.108[0.045+0.023(280) +0.017(280)^2] \times 10^{-5}\}$

= 1.730 KJ /mol

$Q_C = \Delta H_L - \Delta H_V$

= (16.280 – 1.730)

= 14.55 KJ/mol

$\Delta H_f + Q_B = \Delta H_w + \Delta H_D + Q_c$

- ⇨ $606.592 + Q_B = 294.296 + 312.296 + 14.55$
- ⇨ $Q_B =$ 14.55 KJ/mol

Let m be the amount of water required at condenser.

$m \int_{280}^{281} 75.4\, dT = 312.296$

- ⇨ m = 4.1384 mol/hr

Let, m be the amount of steam required in the reboiler

$m\lambda = 294.296$

- ⇨ $m = \frac{294.296}{4.1384}$
- ⇨ m = 71.12 Kmol/hr

Table: Energy Balance over Distillation Column:

Input	KJ/mol	Output	KJ/mol
Feed	606.592	Top Product C_2H_2O	294.296
Reboiler duty	14.55	Bottom product H_2O	312.296
		Condenser Duty	14.55
Total	621.142	Total	621.142

Table 23: Energy Balance for Distillation Column

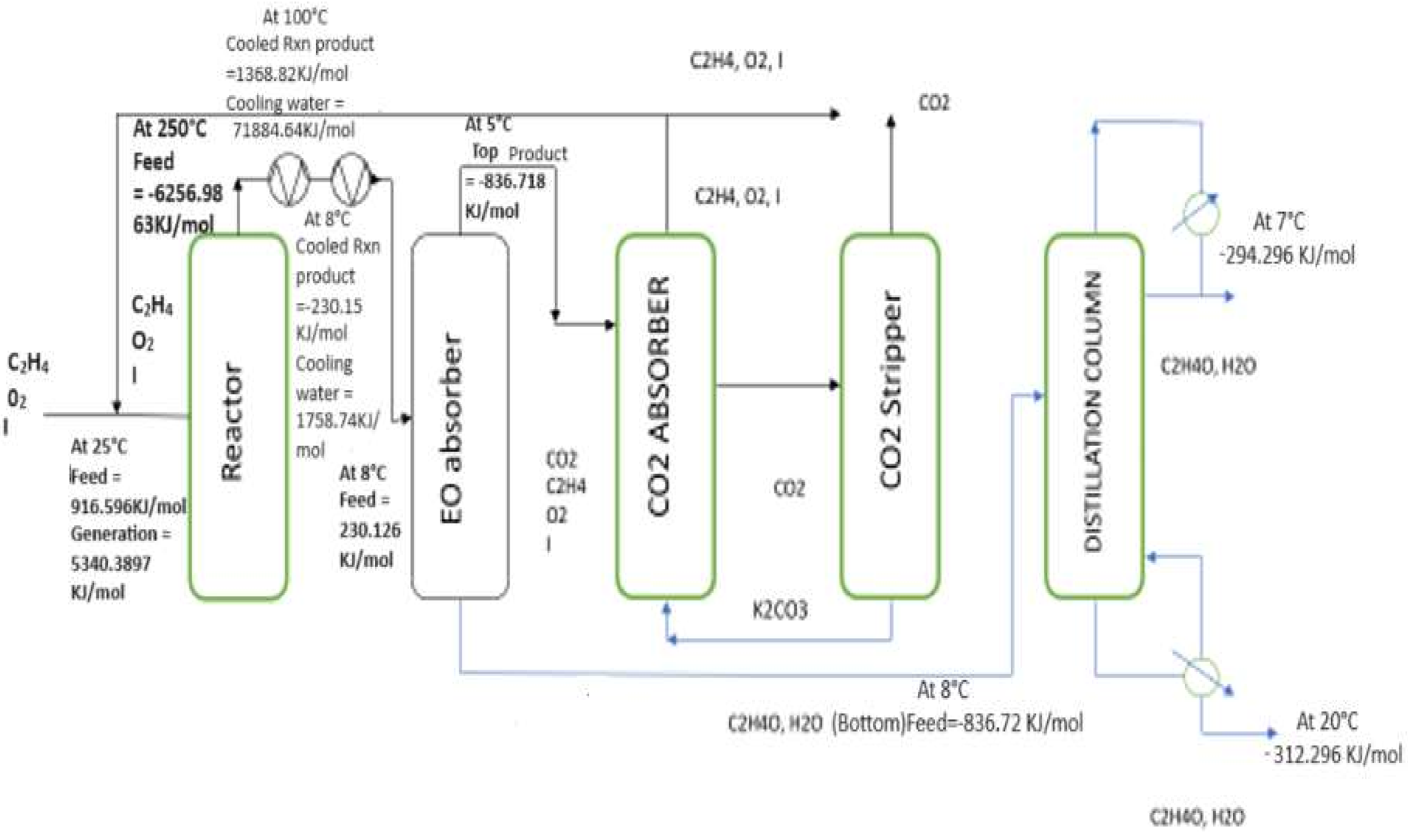


Fig: Flowchart with Energy Balance

CHAPTER 10: DESIGN OF HEAT EXCHANGER AND CO_2 ABSORBER

DESIGN OF HEAT EXCHANGER 1:

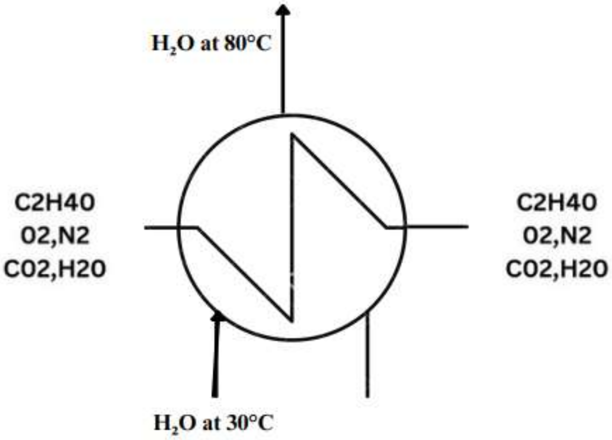


Figure 17: Heat Exchanger 1

Assumption of U_d = 100 and R_d= 0.0001 is taken (DQ kern)

- Allowable pressure drop on each stream is 10 psi.

Mixed feed consists of the following components:

Component	Mass fraction
C2H4	0.032
O2	0.080
C2H4O	0.050
CO2	0.10
H2O	0.041
N2	0.692

Table 24: Components of the Mixed Feed

Calculations of Cp, u, k values:

Cp = 0.9758* 0.032+ 0.080* 0.9066+ 0.050*0,8693 +0.10* 1.66+ 0.041* 0.8939+ 0.7960*0.692

= 0.89 Btu/ lb ^{0}F

μ= 0.00196+ 0.005592+ 0.00143+ 0.00565+ 0.002061+ 0.0002304

= 0.016 Cp

K= 0.00244+ 0.005368+ 0.007825+ 0.00754+ 0.0175+ 0.0397

= 0.08 Btu/hr Ft^2 ^{0}F/Ft

Shell side	Tube side
ID= 21.1/4 Baffle space = 12 inch	Number and length = 364, 16' 0 '' OD, BWG, Pitch = ¾ inch, 16 BWG, 15/16 Inch, triangular pitch
Passes = 1	Passes = 2

Step 1:

Hot fluid (mixed feed):

T1 = 482 ^{0} F T2 =212^{0}F

T$_{avg}$ = 482+ 212 /2

=347^{0}F

Cp$_{hot}$ = 0.89

Cold fluid (water):

t 1= 86^{0}F t 2= 176^{0}F

t avg = 131^{0}F

Cp$_{col}$d = 1.01 Btu/ lb^{0}F (FIG 2 DQ Kern)

Step 2: Heat Balance

Q_{hot} = m Cp dT

= 116621.8092 * 0.89* 270 J/ hr

= 61653285.65 Btu/ hr

Q_{cold}= mCp dT

= 678253.96 * 1.01* 90

= 61653284.96 Btu/ hr

LMTD = 306- 126 / ln (306/126)

= 180/ 0.887

= 202. 93

LMTD Correction Factor:

R= T1- T2 / t2 -t1

= 270/ 99

=2.72

S= t2-t1/ T1-t1

=0.244

Ft = 0.87 (fig 18 DQ Kern)

Δt = LMTD * Ft

= 176.54 ^{0}F

A = Q/ Ud *LMTD

= 61653285.65/ 100*176.54

= 3492. 31 ft^2 > 200 ft^2

Since area is greater than 200 ft^2 therefore Shell and tube heat exchanger is used. Considering 1-2 Shell and tube H.E.,

Step 3: Caloric / Average Temperature

Viscosity at cold end temperature

μ at 212^0F = 0.016 < 1 Cp

μ at 86^0F = 0.85 < 1 Cp (fig 14, DQ kern)

hence calorific temperature is used.

Step4 : Property Table

Property	Hot fluid (347^0F)	Cold fluid (131^0F)
Cp (figure 2, DQ Kern)	0.89	1.01
μ (fig 15, DQ Kern)	0,016	0.85
K (table 5) DQ Kern	0.08	0.881
S	1.795	1
p	104.5	62.5

Table 25: Property Table

Step 5: h_0 and h_i Calculation

Hot fluid (shell side), mixed feed	Cold fluid (tube side), water
Flow area, a_s = ID*C''*B /144*Pt = 21.25*0.188*12/ 144*0.75 = 0.443 ft^2 Mass velocity, Gs = w/ a_s = 116621.8092 / 0.443 = 263254.64 lb/hr. ft^2 De= 0.55/12 = 0.0458 ft (fig 28)	$A_{t'}$ = 0.302 ft^2 (table 10) a_t = Nt* a_t' / 144 n = 364*0.302 / 144*2 = 0.381 ft^2 G_t = w/ a_t = 678253.96/ 0.381 = 1780194.12 lb/ hr ft^2

Re = D Gs / μ = 0.0458* 263254.64/ 0.016 = 753566.4308 From figure 28 DQ Kern, J_H = 590 ho = J_H*K /De (Cp *μ/k) $^{1/3}$ =590*0.08/0.0458 (0.89*0.038/0.08)$^{1/3}$ = 775.68	Vt = Gt/ 3600*p = 1780194.12 / 3600*62.5 = 7.91 ft/hr D= 0.620/12 = 0.051 ft (table 10) Re_t = D* Gt / μ = 90789.90/ 0.85* 2.42 = 44137.04 hi = 1510 (fig 25, DQ Kern) hi_o = hi *ID/ OD = 1510* 0.62/ 0.75 = 1248.26

Table 26: h_0 and h_i Calculation

Step 6: Clean Overall Coefficient

$$U_c = \frac{h_0 * h_{i0}}{h_0 + h_{i0}}$$

$$= \frac{968250.3168}{2023.94} = 478\frac{Btu}{hr}.ft\text{^}2°\mathrm{F}$$

External surface, a'' = 0.1963 ft^2/ft (table 10 DQ kerm)

Area, A= 364* 16 *0.1963 = 1143.25 ft^2

Step 7: Overall coefficient

$$U_{d\ corrected} = \frac{61653285.65}{1143.25 * 176.54}$$

= 305.47

Step 8: Dirt Factor (R_d)

R_d = $(U_c + U_d)/((U_c * U_d)$

= (478+305.47)/ 146014.66

= 0.005 Btu / hr ft^2 °F

Therefore, R_d calculated is greater than the theoretical R_d

Step 9: Calculation of pressure drop

Shell side	Tube side
R_{es} = 753566.430 D_s = 21.25 / 12 = 1.77 f = 0.01 ft^2/inch^2 (fig 29) $\emptyset_s$=1 No. of crosses = N+1 = 12L/ B = 12*16/12 = 16 $\Delta P_s = \frac{f * G_s^2 * D_s * (N+1)}{5.22 * \ 10^{10} * D_e s \emptyset_s}$ $= \frac{0.01*(263254.64^2*1.77*16}{5.22*10^{10}*0.0458*1.795*1}$ =4.753 Psi < 10 Psi	R_{et} = 44137.04 f= 0.0016 (fig 29) $\Delta P_t = \frac{f * G_t^2 * L * n}{5.22 * \ 10^{10} * D_e s \emptyset_t}$ $= \frac{0.016*(1780194.12)^2*16*2}{5.22*10^{10}*0.051*1*1}$ = 0.632 Psi $\frac{V_t^2}{2g'}$ = 0.023 (fig 27 DQ kerm) $\Delta P_s = \frac{4nV_t^2}{s * 2g'}$ $= \frac{4*2*0.023}{1}$ = 0.184 Psi ΔP_T = 0.184 + 0.632 = 0.816 Psi < 10 Psi

Table 27: Calculation of Pressure Drop

Design of CO2 Absorber:

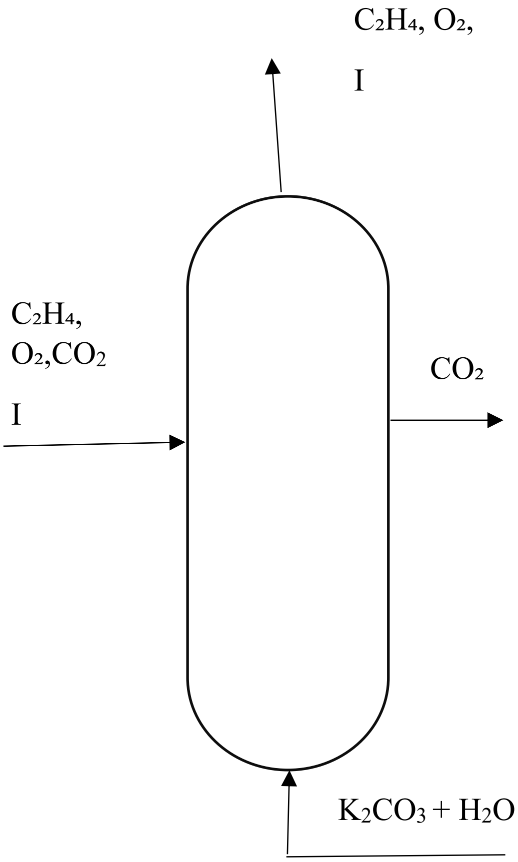


Figure 18: CO_2 Absorber

Feed rate, F = 106470.0253 kg/hr

= 234726.2263 lb/hr

Molecular Weight of gas mixture entering = 29.5328 kg/mol

Let GL/GS = 2:1

Density of gas mixture, $\rho_G = \frac{P + m_{avg}}{RT}$

Pressure, P = 20 bar = 19.73 atm

Temperature, T = 8 ˚C = 281 K

$= \frac{19.73 * 29.5329}{0.0821 * 281} = 25.257 \text{ kg/m}^3$

$= \frac{25.257 * 2.2046}{(3.2084)3} = 1.685 \text{ lb/ft}^3$

The K_2CO_3 solution is assumed to be 20 % concentrated

Density for K_2CO_3 solution, $\rho_L = 1.22 \text{ g/cm}^3$

$= 76.162 \text{ lb/ft}^3$

Flow parameter $= \frac{2}{1} \sqrt{\frac{\rho G}{\rho L}}$ $\circ$

$= \frac{2}{1} \sqrt{\frac{1.685}{76.162}} = 0.148$

For Pall Ring, 1 inch, Fp = 56 ft^{-1}(From Table 10.6-1, Transport processes and separation process principles By Christie John Geankolis)

Pressure drop, $\Delta P_{flood} = 0.115\ (56)^{0.7}$

$= 1.925$inch H2O /ft

Capacity parameter = 1.48 (From Figure 10.6-5, Transport processes and separation process principles

By Christie John Geankolis)

Capacity parameter $= Vg \left[\frac{1.685}{76.162 - 1.685} \right]^{0.5} * (56)^{0.5} * (1.393)^{0.05}$

$1.38 = Vg * 0.1504 * 7.4893 * 1.0167$

$Vg = 1.206$

Now, $G_G = Vg * \rho_G$

$= 1.206 * 1.685$

$= 2.03211$ lb/s ft^2

Cross Sectional Area, $A = F / G_G$

$= \frac{234726.2263}{2.032*3600}$ ft^2

$= 32.08746$

Area, $A = \prod / 4\ D^2$

$D^2 = 40.87$

$D = 6.393$ ft $= 1.948$ m

CHAPTER 11: CONCLUSION

In conclusion, ethylene oxide production involves a complex manufacturing process that is essential for meeting the demand of various industries. The most common method for producing ethylene oxide is the direct oxidation of ethylene using oxygen or air as a catalyst. This process takes place in a high-pressure reactor, typically using a silver-based catalyst, which facilitates the reaction between ethylene and oxygen.

During the oxidation reaction, ethylene and oxygen react to form ethylene oxide. However, the reaction is highly exothermic and can lead to temperature spikes, which need to be carefully controlled to avoid safety hazards. The use of a catalyst helps in achieving the desired reaction rates while minimizing unwanted side reactions.

As the industry progresses, efforts are being made to develop more sustainable and environmentally friendly methods for ethylene oxide production. These include exploring alternative catalysts, optimizing reaction conditions, and integrating energy-efficient processes. By combining technological advancements with a commitment to safety and sustainability, the future of ethylene oxide production holds the potential to meet global demands while minimizing its impact on the environment.

CHAPTER 12: REFERENCES

---

1. https://www.sciencedirect.com/science/article/abs/pii/S0959652620328183
2. Handbook of Petrochemicals and processes by G. Margaret Wells
3. https://scholar.google.com/scholar?hl=en&as_sdt=0%2C5&q=Ethylene+Oxide+SIEGFRIED+REBSDAT%2C+Winh%E2%82%ACoring%2C&btnG=#d=gs_qabs&t=1708330380941&u=%23p%3DdW2AfmTSLuIJ
4. https://scholar.google.com/scholar?hl=en&as_sdt=0%2C5&q=ethylene+oxide+production+by+direct+oxidation+&oq=#d=gs_qabs&t=1708330753005&u=%23p%3Dqh9LMfawyxYJ
5. https://scholar.google.com/scholar?hl=en&as_sdt=0%2C5&q=ethylene+oxide+production+by+direct+epoxidation+&btnG=#d=gs_qabs&t=1708330871978&u=%23p%3DAaIQKMMUenQJ
6. https://patents.google.com/patent/CN104693147A/en
7. Perry’s Chemical Engineers’ Handbook