

MANUFACTURE OF ETHYLENE OXIDE

Ethylene oxide has been produced commercially by two basic routes:

1. From ethylene chlorohydrin.
2. Direct oxidation process.

The chlorohydrin process was first introduced during World War I in Germany by Badische Anilin-und Soda-Fabrik (BASF). The process involves the reaction of ethylene with hypochlorous acid followed by dehydrochlorination of the chlorohydrin with lime to produce ethylene oxide and calcium chloride. Union Carbide Corp. was the first to commercialize this process in United States. The chlorohydrin process is not economically competitive, and was quickly replaced by the direct oxidation process as the dominant technology. At 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 high purity oxygen stream (>98 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. All the ethylene oxide plants that have been built during the last 15 years were oxygen-based processes and a number of plants were converted from the air to the oxygen-based process during the same period. The total world production capacity of ethylene oxide in 1992 was about 9.6×10^6 metric tons. Most of the ethylene oxide produced is consumed by its producers in making derivatives.

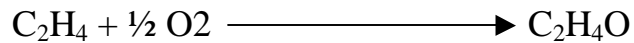
The chosen process for this design thesis is the oxygen-based oxidation process, because this is the latest process for the production of ethylene oxide production.

DIRECT OXIDATION PROCESS:

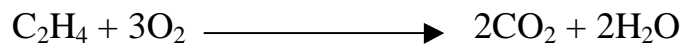
The phenomenal growth in United States and world ethylene oxide production capacity since 1940 and the market trend toward larger single-train plant is chiefly due to the commercial success of the direct oxidation process. Compared to the chlorohydrin process, direct oxidation eliminates the need for 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. 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 mol% of the ethylene to carbon dioxide and water. Consequently the operating conditions must be carefully controlled to maximize selectivity.

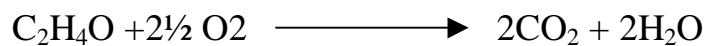
All the ethylene oxide plants are based on the original process chemistry discovered by Lefort in 1931.



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



Or by further oxidation of ethylene oxide:



To prevent the further oxidation of ethylene oxide, the ethylene conversion is typically between 20-30% for ethylene oxide.

In addition to ethylene oxide, carbon dioxide, water, small quantities of acetaldehyde and traces of formaldehyde are also produced. In this calculation this is neglected and assumed to go with the bottom products.

The total percentage of production of these compounds is 0.2% of the total ethylene oxide produced.

A large amount of heat is released by the ethylene oxide reactions. At 600 K, each Kg of ethylene converted to ethylene oxide releases 3.756 MJ; each Kg of ethylene converted to carbon dioxide and water releases 50.68 MJ. Energy recovery and integration is a prime concern in process design.

PROCESS DESCRIPTION:

Ethylene (95-98% purity) and oxygen (air with 95 mole % of oxygen) are mixed in a ratio of 1:10 by weight and passed over a catalyst consisting of silver oxide deposited on an inert carrier such as corundum. Generally an anti catalyst such as ethylene dichloride (about 2% based on the weight of ethylene) is added to the ethylene feed to suppress the formation of carbon dioxide. As an alternative vent gases from the absorber may be recycled to the reactor in such quantity as to keep the ethylene concentration in the feed at 3-5%. At a pressure of 4-5 atmosphere and temperature of 270-300°C, when a contact time of 1 sec is used, about 50 % of ethylene is converted. 25% of the ethylene is converted to ethylene oxide.

The effluent gases from the reactor are washed with water under pressure in an absorber. The ethylene is absorbed and sent to a desorber to desorb the water, which is used for the absorption. This water is recycled.

The overhead product from the desorber is sent to a steam stripper to remove the dissolved gases. The water- ethylene oxide mixture with small amount of ethylene and other impurities are fed to a fractionating column to purify the ethylene oxide to 99 mole%.

Commercial processes operate under recycle conditions in a packed bed multitubular reactor. The reactor is of shell and tube type comprised of several thousand mild steel or stainless steel tubes, 20-50 mm inside diameter. The reactor can be either oil or boiling water-cooled. These tubes are filled with a silver based catalyst ca 3-10 mm diameter supported on a carrier material with surface area usually $< 1\text{m}^2/\text{g}$. The yield (moles of product formed per moles of ethylene consumed in the process) is normally 70-80% depending on catalyst type, per pass conversion, reactor design and normally a large number of other process variables.

OXYGEN BASED DIRECT OXIDATION

Even though the fundamental reaction and the ultimate results are the same there are substantial differences in air and oxygen based processes. Virtually all the differences arise from the change in the oxidizing agent from air to pure oxygen (95 mole% O_2). Due to the low per pass conversion, the need for complete removal for ethylene oxide by absorption, and the accumulation of nitrogen in the cycle, the air process requires a substantial

purge stream. As a direct consequence of this air process requires the staged reaction- absorption system. 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 unreacted ethylene. This eliminates the need for purge reactor in the oxygen-based process. However the volume of the carbon dioxide formed is about 2 times the volume of the ethylene reacted at a catalyst selectivity of 70-80%. This CO₂ must be eliminated on a continuous basis in order to control its concentration at an acceptable level in the cycle. Concentrations of CO₂ much in excess of 15-mole% adversely affect the catalyst selectivity. Therefore in oxygen-based process the recycled gas is treated in a CO₂ removing tower before it is send back to the reactor. The operation of the main reactor can be at much higher ethylene concentration than that possible in air-based process is much smaller than an air-based unit. The high ethylene concentration improves the catalyst selectivity because the per pass conversions are lower for a given ethylene oxide production.

In the flow sheet of the shown the process is an oxygen-based process. Ethylene, oxygen, and the recycle gas stream are combined before entering the tubular reactors. The basic equipment used in this process is same as that used in air-based process. The purge reactor is not used in this process.

PROCESS TECHNOLOGY CONSIDERATIONS

Innumerable complex and interacting factors ultimately determine the success or failure of a given ethylene oxide process. Those aspects of process technology of the oxygen-based oxidation system are reviewed below.

Ethylene oxide catalyst: Of all the factors that influence the utility of the direct oxidation process for ethylene oxide, the catalyst used is of the greatest importance.

It is for this reason that catalyst preparation and research have been considerable since the reaction was discovered. There are four basic components in commercial ethylene oxide catalyst: the active catalyst metal; the bulk support; catalyst promoters that increase selectivity and/or activity and improve catalyst life; and inhibitors or anticycatalysts that suppress the formation of carbon dioxide and water without appreciably reducing the rate of formation of ethylene oxide.

The components of the catalyst are:

1. The active catalyst metal- silver. A variety of methods are used for the preparation of the silver based catalyst on relatively inert supports.
2. Bulk support- the supports used commercially are alumina (α -alumina), silicon carbide. Other supports are glass wool, quartz, carborundum, and

ion-exchange zeolites. The physical and chemical properties of the support strongly dictate the performance of the finished catalyst. The surface area, porosity, and pore size of the support influence the size of the silver particles on the support and, therefore, affect the performance of the final catalyst. High surface supports (3-100 m²/g) generally yield poor ethylene oxide catalysts presumably because ethylene reacts in the pores from which ethylene oxide is released slowly. The combination of slow product release and poor heat conductivity of high surface area supports is claimed to result in the combustion of ethylene oxide.

3. Promoters- alkaline earth metals. Silver alone on a support does not give rise to a good catalyst. However, addition of minor amounts of promoter enhances the activity and the selectivity of the catalyst, and improves its long-term stability. Excess addition lowers the catalyst performance. The most commonly used promoters are alkaline earth metals, such as calcium or barium, and alkali metals such as cesium, rubidium, or potassium. Using these metals in conjunction with various counter anions, selectivities as high as 82-87% were reported.
4. Inhibitors- organic halides. Many organic compounds, especially the halides, are very effective for suppressing the undesirable oxidation of ethylene to carbon dioxide and water, although not significantly altering

the main reaction to ethylene oxide. These compounds referred to as catalyst inhibitors, can be used either in the vapour phase during the process operation or incorporated into the catalyst manufacturing step. Important gas phase inhibitors are ethylene dichloride, ethylene dibromide, other alkyl halides, aromatic hydrocarbons, amines, and organometallic compounds. In a study of the effect of ethylene dichloride on catalyst activity, it was found that small amounts improved catalyst performance. In this design thesis the inhibitor suggested is ethylene dichloride.

Operating pressure: Operating pressure has a marginal effect on the economics of the ethylene oxide process. High-pressure increases production due to higher gas density, increases heat transfer, increases ethylene oxide and carbon dioxide recovery in the absorber, and lower the compression costs. Also, since the total number of moles decreases in the formation of ethylene oxide from ethylene and oxygen, high pressure is consistent with high conversion. However high pressures reduce the flammable limit of the process gas as well as increase equipment costs. Typical pressures are 4-5 atmospheres.

Temperature and Thermal effects: Temperature is used to control two related aspects of the reaction: heat removal from the reactor bed and

catalyst operating temperature. The reactor temperature is controlled through the use of a heat-transfer fluid on the reactor shell. The coolant used in most recent designs is boiling water. Boiling water provides good heat transfer and improved safety over previous reactor designs using either boiling or circulation organic heat transfer fluids. Control of the catalyst operating temperature is necessary to prevent catalyst damage such as sintering or tube damage resulting from excessive temperatures in the catalyst bed. Localized hot spots of 100-300° C above the coolant temperature can form in the catalyst bed without adequate temperature control.

Heat removal from the reactor is necessary for stable operation. The reactor stability is affected by the internal temperature profile in the tubular catalyst bed.

Raw Material Purity Requirements: The oxygen process has four main raw materials: oxygen, ethylene, nitrogen (cyclic diluent), and inhibitor ethylene dichloride. The purity requirements are established to protect the catalyst from damage due to poisons or thermal runaway, and to prevent the accumulation of undesirable components in the recycle gases. The latter can lead to increased cycle purging, and consequently higher ethylene losses. Typical ethylene specifications call for a minimum of 99.85-mol% ethylene. The primary impurities are usually ethane and methane. A methane limit is

largely unnecessary; however, care should be taken to restrict the amount of ethane since high ethane concentration will lead to increased chloride inhibitor concentration, which adversely affects the product quality, catalyst life and materials of construction. Impurities that strongly affect catalyst performance and reactor stability include acetaldehyde, propylene, hydrogen, and sulphur. Acetylene causes catalyst coking at very low concentrations. Carbonaceous deposits can also be caused by heavy hydrocarbons if present. Propylene is more reactive than ethylene and will oxidize to a wide range of products, including aldehydes that lower the product quality. Hydrogen and carbon monoxide can be lead to hot spotting of the catalyst, and sulphur is a nonreversible poison for silver-based catalyst.

Oxygen must be 95 mol% pure and rest is assumed to be nitrogen. Presence of argon is assumed to be negligible. Organic chloride specifications are less critical since the flows are significantly less.

Ethylene Oxide Recovery: An economic recovery scheme for a gas stream that contains less than 3 mol% ethylene oxide must be designed. It is necessary to achieve nearly complete removal since any ethylene oxide recycled to the reactor would be combusted or poison the carbon dioxide removal solution. Commercial designs use a water absorber followed by

vaccum or low pressure stripping of ethylene oxide to minimize oxide hydrolysis.

Ethylene oxide purification: The main impurities in ethylene oxide are water, traces of carbon dioxide, acetaldehyde and formaldehyde. The water and heavy ends are removed in the distillation column, which works under atmospheric pressure. Acetaldehyde and formaldehyde are assumed to be present in PPM level.

END USES OF ETHYLENE OXIDE

Use Pattern

This estimate was made in the year 1995.

Use	Percent
Ethylene glycol	64
Glycol ethers and polyglycols	11
Detergents	10
Ethanolamines	8
Acrylonitrile	5
Miscellaneous	2
	<hr/>
	100

Ethylene oxide is an excellent fumigant and sterilizing agent. Ethylene oxide is used as an antimicrobial pesticide to fumigate. Species and to sterilize medical devices, such as sutures, bandages, endoscopes and cardiac pacemakers. Most medical devices in the USA are sterilized using EO. Ethylene oxide sterilization process requires relatively low temperatures and pressures, and does not damage the materials or packaging being sterilized.

Ethylene oxide sterilant gases are supplied as liquefied compressed gases, either pure or as a mixture with a flame retardant. When supplied as a

pure gas, the ethylene oxide is shipped in special insulated containers. For safety reasons, nitrogen gas is added to the vapour phase up to a total pressure of 345 Kpa (50 psig) at 21°C. When used in a sterilizing chamber, the flammability of ethylene oxide is usually controlled by purging the sterilization chamber with nitrogen gas at the beginning and the end of the sterilization process. In some cases, the effects of a potential deflagration are moderated by operating under great vacuum or, in the case of small hospital sterilizers, by using very small quantities of ethylene oxide.

Ethylene oxide has been studied for use as a rocket fuel and as a component in munitions. It has been reported, ethylene oxide to be used as a fuel in FAE (fuel air explosive) bombs.

HEALTH AND SAFETY FACTORS

Mutagenicity, Neurotoxicity & General Toxicological factors of Ethylene oxide.

TOXICOLOGY:

An excellent review of the toxicity and health assessment of ethylene oxide has been compiled. Ethylene oxide (EO) can be relatively toxic as both a liquid and gas. Inhalation of ethylene oxide in high concentrations may be fatal. Estimates of lethal ethylene oxide inhalation levels in animals

depend on the duration of exposure. The reported 4-h LC50 values for rats, mice, and dogs are 1460, 835, and 960 ppm, respectively. More recent information indicates that the 1-h LC50 in rats is approximately 5000 ppm.

Inhalation exposure to high concentrations of ethylene oxide has been reported to result in respiratory system irritation and edema. Depending on the degree of exposure, there may be stinging of the nose and throat, coughing, and chest tightness. Also, exposure may cause lung injury and delayed onset of pulmonary edema. In long-term studies of animals exposed to less than 100 ppm of ethylene oxide and in human studies, no evidence of injury has been reported for the cardiovascular system, liver, or kidney. There is some evidence that occupational exposure to high levels of ethylene oxide can result in cataracts.

Neurological effects have also been reported in association with recurrent human and animal inhalation exposures to ethylene oxide. Again, depending on the degree of exposure, headache, nausea, vomiting, diarrhea, dizziness, loss of coordination, convulsion, or coma may occur. The onset of illness is rapid in severe exposures, but may be delayed after moderate exposure.

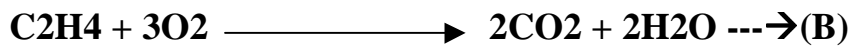
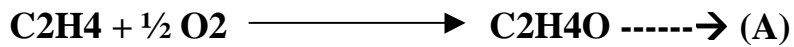
In the reports of human peripheral neurotoxic effects or central nervous system toxicity, most cases have shown a marked improvement on removal from further exposure.

Ethylene oxide has been shown to produce mutagenic and cytogenic effects in a variety of test systems. An increased frequency of chromosomal aberrations in peripheral lymphocytes of monkey exposed to ethylene oxide for 104 weeks has been reported. In mice, it is an effective inducer of chromosome breaks leading to dominant-lethal mutations.

THERMODYNAMICS AND KINETICS OF

REACTIONS

The two reactions taking place in the manufacture of ethylene oxide from ethylene in direct oxidation is given below.



Temperature range of the reaction = 250-300°C

Pressure range in the reactor = 4- 5 atmospheres.

Table: 2.1 Specific Heat Data of the components:

$$C_p/R = A + B*T + C*T^2 + D*T^{-2}$$

T is the temperature in Kelvin.

Component	A	B*10 ³	C*10 ⁶	D*10 ⁻⁵
C₂H₄	1.424	14.394	-4.392	-----
C₂H₄O	-0.385	23.463	-9.296	-----
O₂	3.639	0.506	-----	-0.227
CO₂	5.457	1.045	-----	-1.157
H₂O	3.470	1.450	-----	0.121

Table: 2.2 Energy Data of components at temperature of 298 K:

Component	$\Delta H^{\circ}f$ (J/ K mole) 10^7	$\Delta S^{\circ}f$ (J/ K mole K) 10^5	$\Delta G^{\circ}f$ (J/ K mole) 10^7
C₂H₄	5.2510	2.1920	6.8440
C₂H₄O	-5.2630	2.4299	-1.3230
O₂	0	2.054	0
CO₂	-39.3510	2.1638	-39.4370
H₂O	-24.1814	1.8872	-22.850

The enthalpy of formation at the reaction temperature can be calculated using the following equations.

$$\Delta H_T = \Delta H^{\circ}f_{298K} + R \int \Delta C_p/R dT \rightarrow (1)$$

Where, ΔH_T is the enthalpy of formation of the reaction at the reaction temperature T is the temperature and R is the universal gas constant. The integration limits are from 298 K- T K.

$$\Delta H_T = \Delta H^{\circ}f_{298K} + R [\Delta A * T + \Delta B * T^2/2 + \Delta C * T^3/3 - \Delta D * T^{-1}] \rightarrow (2)$$

Entropy of the reaction is calculated using the following equations.

$$\Delta S_T = \Delta S^{\circ}f_{298K} + R \int \Delta C_p/R * 1/T * dT \rightarrow (3)$$

Where, ΔS_T is the entropy of the reaction at the reaction temperature. T is the temperature and R is the universal gas constant. The integration limits are from 298 K- T K.

$$\Delta S_T = \Delta S^\circ_{298K} + R [\Delta A \cdot \ln(T) + \Delta B \cdot T + \Delta C \cdot T^2/2 - \Delta D \cdot T^{-2}/2] \rightarrow (4)$$

Table: 2.3 Thermodynamic data for the reaction: A

Temperature, K	ΔH , J/K mole 10^{-6}	ΔS , J/K mole-K 10^{-3}	ΔG , J/K mole 10^{-6}
523	-106.47	-80.10	-64.578
533	-106.49	-85.94	-60.7
543	-106.51	-86.10	-59.76
553	-106.54	-86.13	-58.91
563	-106.54	-86.21	-58.00
573	-106.55	-86.28	-57.11

Calculation for the table: 2.3

$$\begin{aligned} \Delta H^\circ_{298K} &= \Delta H^\circ_{298K} \text{C}_2\text{H}_4\text{O} - [\Delta H^\circ_{298K} \text{C}_2\text{H}_4 - 1/2 \cdot \Delta H^\circ_{298K} \text{O}_2] \\ &= (-5.2630 - 5.2510 - 0) \cdot 10^7 \\ &= \mathbf{-105.14 \cdot 10^6 \text{ J/K mole}} \end{aligned}$$

$$\begin{aligned} \Delta S^\circ_{298K} &= \Delta S^\circ_{298K} \text{C}_2\text{H}_4\text{O} - [\Delta S^\circ_{298K} \text{C}_2\text{H}_4 - 1/2 \cdot \Delta S^\circ_{298K} \text{O}_2] \\ &= (2.4299 - (2.1920 - 1/2 \cdot 2.0504)) \cdot 10^5 \end{aligned}$$

$$= -78.73 * 10^3 \text{ J/K mole} - \text{K}$$

$$\Delta H_{523} = \Delta H^\circ_{298\text{K}} + R \int \Delta C_p/R dT$$

The temperature limit is from 298 K- 523K. On integration and supplying the limits,

$$\begin{aligned} \Delta H_{523} = & [-105.14 * 10^6 + 8314 * (-3.6285 * (523 - 298) + (8.816 * 10^{-3}/2) \\ & * (523^2 - 298^2) - (4.904 * 10^{-6} * ((523^3 - 298^3)/3) - 0.2207 * 10^5 * (1/523 - \\ & 1/298)] \\ & = -106.47 * 10^6 \text{ J/ K mole.} \end{aligned}$$

$$\Delta S_{523} = \Delta S^\circ_{298\text{K}} + R \int \Delta C_p/R * 1/T dT$$

The temperature limit is from 298 K- 523K. On integration and supplying the limits,

$$\begin{aligned} \Delta S_{523} = & [-78.73 * 10^3 + 8314 * (-3.6285 * (\ln(523) - \ln(298)) + (8.816 * 10^{-3}) \\ & * (523 - 298) - (4.904 * 10^{-6} * ((523^2 - 298^2)/2) - (0.2207/2) * 10^5 * (1/523^2 - \\ & 1/298^2)] \\ & = -80.10 * 10^3 \text{ J/ K mole} - \text{K} \end{aligned}$$

$$\Delta G = \Delta H - T * \Delta S$$

$$= -106.47 * 10^6 + 523 * 80.10 * 10^3$$

$$= -64.578 * 10^6 \text{ J/K mole}$$

Table:2.4 Thermodynamic data for the reaction: B

Temperature, K	ΔH , J/K mole 10^{-9}	ΔS , J/ K mole- K 10^{-3}	ΔG , J/ K mole 10^{-9}
523	-1.324	-31.85	-1.307
533	-1.324	-32.00	-1.307
543	-1.324	-32.16	-1.3065
553	-1.324	-32.32	-1.3061
563	-1.324	-32.48	-1.3057
573	-1.324	-32.64	-1.3053

Calculation for the table: 2.4

$$\Delta H^{\circ} f_{298K} = 2 * \Delta H^{\circ} f_{298K} \text{ CO}_2 + 2 * \Delta H^{\circ} f_{298K} \text{ H}_2\text{O} - [\Delta H^{\circ} f_{298K} \text{ C}_2\text{H}_4 - 1/2 * \Delta H^{\circ} f_{298K} \text{ O}_2]$$

$$\Delta H^{\circ} f_{298K} \text{ O}_2]$$

$$= 2 * -39.3510 * 10^7 + 2 * -24.1814 * 10^7 - [5.2630 * 10^7 + 2 * 0]$$

$$= \mathbf{-1.323 * 10^9 \text{ J/ K mole}}$$

$$\Delta S^{\circ} f_{298K} = 2 * \Delta S^{\circ} f_{298K} \text{ CO}_2 + 2 * \Delta S^{\circ} f_{298K} \text{ H}_2\text{O} - [\Delta S^{\circ} f_{298K} \text{ C}_2\text{H}_4 - 1/2 * \Delta S^{\circ} f_{298K} \text{ O}_2]$$

$$\Delta S^{\circ} f_{298K} \text{ O}_2]$$

$$= 2 * 2.1368 * 10^5 + 2 * 1.8872 * 10^5 - [2.1920 * 10^5 +$$

$$3 * 2.0504 * 10^5]$$

$$= -29.52 \times 10^5 \text{ J/ K mole} - \text{K}$$

$$\Delta H_{523} = \Delta H^\circ_{298\text{K}} + R \int \Delta C_p/R \, dT$$

The temperature limit is from 298 K- 523K. on integration and supplying the limits,

$$\begin{aligned} \Delta H_{523} = & [-1.323 \times 10^9 + 8314 \times (4.089 \times (523 - 298) - (10.922 \times 10^{-3}/2) \\ & \times (523^2 - 298^2) + (4.392 \times 10^{-6} \times ((523^3 - 298^3)/3) + 1.391 \times 10^5 \times (1/523 - \\ & 1/298)] \\ & = -1.324 \times 10^9 \text{ J/ K mole.} \end{aligned}$$

$$\Delta S_{523} = \Delta S^\circ_{298\text{K}} + R \int \Delta C_p/R \times 1/T \, dT$$

The temperature limit is from 298 K- 523K. On integration and supplying the limits,

$$\begin{aligned} \Delta S_{523} = & [-29.52 \times 10^3 + 8314 \times (4.089 \times (\ln(523) - \ln(298)) - (10.922 \times 10^{-3}) \\ & \times (523 - 298) + (4.392 \times 10^{-6} \times ((523^2 - 298^2)/2) + (1.391/2) \times 10^5 \times (1/523^2 - \\ & 1/298^2)] \\ & = -31.85 \times 10^3 \text{ J/ K mole} - \text{K} \end{aligned}$$

$$\Delta G = \Delta H - T \times \Delta S$$

$$= -1.324 \times 10^9 + 523 \times 31.85 \times 10^3$$

$$= -1.307 \times 10^9 \text{ J/K mole}$$

Calculation of equilibrium constant for the two reactions:

$$\Delta G = -R \cdot T \cdot \ln (K)$$

ΔG & K are the free energy change and equilibrium constants respectively.

For the first reaction; $\Delta G_1 = -R \cdot T \cdot \ln (K_1)$

Therefore;

$$-64.578 \cdot 10^6 = 8314 \cdot 523 \cdot \ln (K_1)$$

$$K_1 = 2.8 \cdot 10^6$$

For the second reaction; $\Delta G_2 = -R \cdot T \cdot \ln (K_2)$

$$-1.307 \cdot 10^9 = 8314 \cdot 523 \cdot \ln (K_2)$$

$$K_2 = \infty$$

Since the equilibrium constant of the second reaction is $K_2 = \infty$. The reaction is irreversible and the conversion is found to be 0.995 or 99.5%.

Calculation of conversions of the reactions:

It is assumed that initially there are 3.5 moles of oxygen and 2 moles of ethylene are present. Initially the product concentration is assumed to be zero.

Table: 2.5 Equilibrium constant and conversion.

Temperat ure	$K_1 * 10^{-6}$	K_2	Conversion, ϵ_1	Conversio n ϵ_2
523	2.8	∞	0.995	0.995
533	0.8	∞	0.995	0.995
543	0.561	∞	0.995	0.995
553	0.367	∞	0.995	0.995
563	0.24	∞	0.995	0.995
573	0.161	∞	0.995	0.995

Table: 2.6 Mole balance table.

Component, (i)	C2H4	C2H4O	CO2	O2	H2O	$\sum v$
(j) 1	-1	1	0	-0.5	0	-0.5
2	-1	0	2	-3	2	0

Mole fraction of the component = $y = (n + n_i * \epsilon_j) / (\sum n + \sum v \epsilon_{i,j})$

$\sum n$ is the total initial number of moles=5.5, n is the initial number of moles of the particular species.

$$y_{C_2H_4} = (2 - \epsilon_1 - \epsilon_2) / (5.5 - 0.5 * \epsilon_1)$$

$$y_{C_2H_4O} = (\epsilon_1) / (5.5 - 0.5 * \epsilon_1)$$

$$y_{O_2} = (3.5 - 0.5 * \epsilon_1 - 3 * \epsilon_2) / (5.5 - 0.5 * \epsilon_1)$$

$$y_{CO_2} = 2 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)$$

$$y_{CO_2} = 2 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)$$

$$K_{y1} = [\text{products}]^a / [\text{reactants}]^b$$

$$= y_{C_2H_4O} / (y_{C_2H_4}) * (y_{O_2})^{0.5}$$

$$= (\epsilon_1) / (5.5 - 0.5 * \epsilon_1) / (\epsilon_1) / (5.5 - 0.5 * \epsilon_1) * [3.5 - 0.5 * \epsilon_1 - 3 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)]^{0.5}$$

$$K_{p1} = K_1 = K_{y1} * P^{\Delta n_1} \text{---} \rightarrow (5)$$

P is the pressure in atmospheres; Δn is the total number of moles.

$$K_{y2} = [\text{products}]^a / [\text{reactants}]^b$$

$$= (y_{CO_2})^2 * (y_{CO_2})^2 / (y_{C_2H_4}) * (y_{O_2})^3$$

$$= [2 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)]^2 [2 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)]^2 / (\epsilon_1) / (5.5 - 0.5 * \epsilon_1) * [3.5 - 0.5 * \epsilon_1 - 3 * \epsilon_2 / (5.5 - 0.5 * \epsilon_1)]^3$$

$$K_{p2} = K_2 = K_{y2} * P^{\Delta n_2} \text{----} \rightarrow (6)$$

From equation (5) & (6)

$$\epsilon_1 = 0.995$$

$$\epsilon_2 = 0.995$$

Theoretical conversion for the reactions is 99%. Bu the practical conversion