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1.0   PROCESS BACKGROUND

1.1. REACTANT DESCRIPTION

Ethylene oxide (C_2H_4O) is a colourless and flammable gas when it under normal condition. It is very toxic and carcinogen. Ethylene oxide production started in 1925 by using the chlorohydrin process and it was improved in 1931 by introducing the much more economic direct catalytic oxidation method. Currently, almost all ethylene oxide production plants are based on the direct oxidation process with air or oxygen using a silver based catalyst. Carbon dioxide and water are produced as by-products of the reaction. Ethylene oxide is an important ethylene based intermediary compound. The primary use for ethylene oxide is in the manufacture of derivatives such as ethylene glycol, surfactants and ethanolamine.

1.2. PRODUCT DESCRIPTION

Ethylene glycol ($C_2H_4(OH)_2$) is a colourless, odourless, low-volatility, low-viscosity, hygroscopic liquid. It is completely miscible with water and many organic liquids. Ethylene glycol produced from ethylene oxide through a catalytic reaction with water at higher temperature resulting in a yield of mono-ethylene glycol (MEG), known as glycol, and the by-products diethylene glycol (DEG) and triethylene glycol (TEG). Ethylene glycol commonly used as an antifreeze agent in automobile cooling systems. Other uses include solvents for the paint and plastic industry, and hydraulic brake fluids. In pure form, it is a colourless clear liquid with a sweet taste and a slightly syrup texture.

1.3. PRODUCT USES

The commercial uses for ethylene glycol take advantage of its reactivity and its ability to depress the freezing point when mixed with water. Uses include:

    a. Polyester/PET resins

    b. All-season automotive antifreeze and coolant formulations

    c. Heat-transfer fluids and industrial coolants

    d. Surface coatings (latex paints, alkyd resins, asphalt emulsions)

    e. Solvents for suspending conductive salts in electrolytic capacitors

    f. Solvent couplers to stabilize against gel formation

    g. Humectants to promote moisture retention in textile fibers, paper, leather, and adhesives

1.4. PROCESS DESCRIPTION

1.4.1. Chemical Reaction

$$CH_2 \overset{O}{\underset{}{\diagup\!\!\!\backslash}} CH_2 + H_2O \xrightarrow{H_2SO_4} \begin{array}{c} CH_2 - OH \\ | \\ CH_2 - OH \end{array}$$
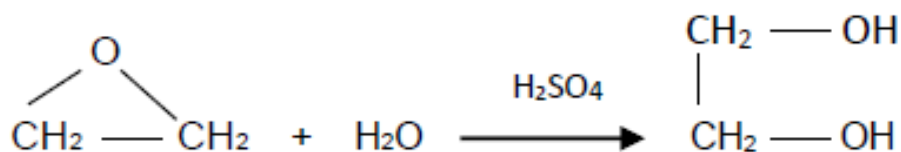
Figure 1 - The Catalytic Process of Ethylene Glycol Production

Ethylene glycol produced from ethylene via the intermediate ethylene oxide. Ethylene oxide reacts with water to produce ethylene glycol according to the chemical equation in figure 1. 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 immediately leads to the formation of ethylene glycol, even at room temperature. The reaction also occurs in the gas phase, in the presence of a phosphoric acid salt as a catalyst.

1.4.2. Side Reaction

The by-products on this reaction are diethylene glycol (DEG) and triethylene glycol (TEG). The side reaction can be reduced if using large amount of excess water feed into the reactor.

1.4.3. Selection of Catalyst

Ethylene oxide reacts readily with water to form ethylene glycol in either an acidic or base solution and slowly reacts with water alone at elevated temperatures. The ethylene glycol in turn may react with more ethylene oxide to form diethylene glycol and this process repeated to form high polymers of high molecular weight. The diluted sulphuric acid is the most suitable catalyst used in this reaction. It is because sulphuric acid is one of the strong acid. The highest yields of ethylene glycol occur at acidic or neutral pH with a large excess of water. Under these conditions, ethylene glycol yields of 90% can be achieved.

1.5. PROCESS FLOW DIAGRAM
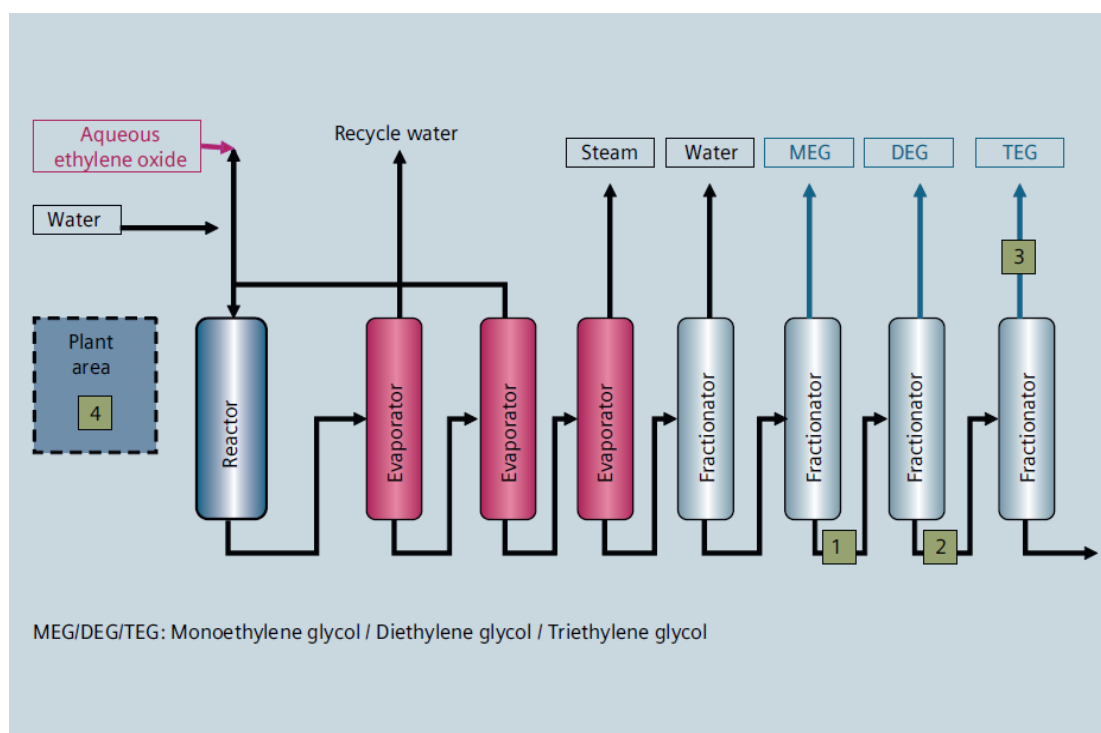
Figure 2 - Process Flow Diagram of Ethylene Glycol Production

The flow diagram of ethylene oxide process based on the hydration of ethylene oxide. The feeds are refined ethylene oxide and pure water. These are mixed with cold recycle water in a feed tank to produce a diluents oxide-water solution containing ethylene oxide. The solution is pumped through preheaters (hot recycle water and steam) into an adiabatic reactor where the ethylene oxide is hydrated to produce ethylene glycols and small amount of di and tri ethylene glycols. When ethylene glycol is the preferred product, the use of a large amount of excess water reduces the formation of heavier glycols.

The glycol reactor is designed to provide sufficient time to react all the ethylene oxide. The reactor pressure controlled at a level that avoids vaporization of ethylene oxide from the aqueous solution and will depend on the initial concentration of the oxide and the reaction temperature. The glycol- water mixture from the reactor feed to the first evaporator that work at a medium-pressure level and is reboiled using high-pressure steam. The following evaporator operates at lower pressure with final stage at low pressure or even under vacuum. The evaporated water is recovered as an overhead condensate is recycled back to the glycol reaction feed tank after heat exchange with cold reactor feed. The concentrated crude glycol solution leaving the final evaporation stripped of its remaining water and light impurities in the light-ends column.

The crude glycols from glycol dehydration are sent the ethylene glycol purification column where ethylene glycol taken off as a side stream where the top product is recycled. Residues from the bottoms of the ethylene glycol column are feed to the diethylene glycol column, where the diethylene glycol product is taken overhead. The diethylene glycol column bottoms are feed to the diethylene glycol recycle column and the remaining diethylene glycol is taken overhead and recycled to the diethylene glycol purification column. Residue from the bottoms of diethylene glycol recycle column are feed to the triethylene glycol purification column where triethylene glycol product is taken over head. The triethylene glycol column bottoms containing tetra ethylene glycols and heavier glycols are sent to waste disposal. Cooled ethylene glycol, diethylene glycol and triethylene glycol products are sent to rundown tanks and from there pumped to final storage.

2.0   REACTOR SELECTION

The production of Ethylene Glycol was carried out in an adiabatic Continuous Flow Stirred Tank Reactor (CSTR) or known as Mixed Flow Reactor (MFR). First and foremost, CSTR or MFR is uniformly mixed, same composition everywhere, within the reactor and at exit. A production from this reactor required an agitation where the reactant enter the feed tank and the reactor effluent is recovered. Continuous Flow Stirred Tank Reactor (CSTR) is a reactor used for continuous production. CSTR is basically ideal for a homogeneous liquid phase reaction and it also can be used for liquid-gas phase process. CSTRs consist of a tank, usually of constant volume and a stirring system to mix reactant together. All calculations performed with CSTR assume perfect mixing, constant density and steady state which is no mass in and out. The reaction rate, r is dependent on the reactant concentration and rate constant, k.
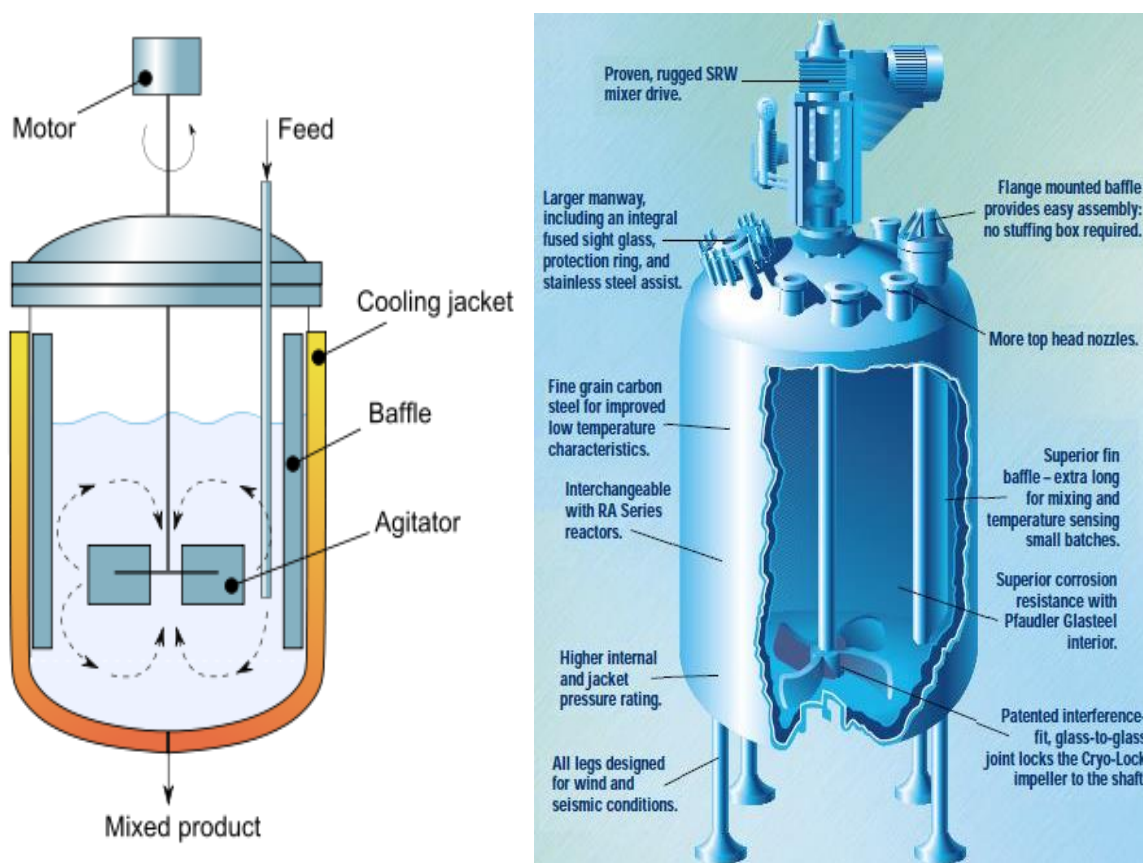

Figure 3 - Model of Continuous Stirred Tank Reactor (CSTR)

Reactor design basically means, which type and size of reactor and method of operation we should employ for a given conversion. Reactor design parameters includes volume of reactor, flowrate of the feed concentration of the feed, reaction kinetic, temperature and pressure. Apart from that, the characteristic of CSTR is based on the high conversion of the reactants in the CSTR reactor, so that cascade of CSTR can be used in a several series of CSTR. In order to minimize the back-mixing and short circuiting, the single vessel is divided into a compartments. An assumption can be made for the CSTR which is the composition and temperature are uniform throughout the tank while the effluent composition is same as in the tank. In contrast CSTR can be classified as an ideal flow type reactor because of the process in the mixed flow, back mix reactor and constant flow reactor.

The advantages of using continuous stirred tank reactor, CSTR are the reactor easy to clean but not as easy as batch reactor. Besides, good temperature control since the tank is covered by the cooling jacket. Other than that, low manpower thus low thus low operating cost. Last but not least, CSTR is highly flexible device as it can operate in parallel and series.

The limitation of CSTR is more complex and expensive than other tubular units. At steady state, the flow rate input must equal to output otherwise the tank will overflow and go empty.

3.0 KINETICS

Ethylene glycol was produced through catalytic reaction of ethylene oxide hydrolysis. Lab scale experiment has been carried out at constant temperature of 85°C to identify the reaction kinetics data. The initial concentration of ethylene oxide used in the experiment is 1 mol/L while water is present in excess. The initial temperature is set to 55°C for the feed fed to reactor. The data collected from the experiment is as tabulated below:

Table 1 - Data Collected From Experiment

Time (min)	Ethylene Glycol Concentration, C_c (kmol/m³)
0	0
0.5	0.145
1.0	0.270
1.5	0.376
2.0	0.467
3.0	0.610
4.0	0.715
6.0	0.848
10.0	0.957

Under the conditions at those at which the reaction is operated on, the reaction is first order in ethylene oxide concentration and apparent zero-order in excess water concentration. Thus, Rate Law:

$$-r_A = kC_AC_B$$

$$-r_A = kC_A$$

$$\frac{-dC_A}{dt} = kC_A$$

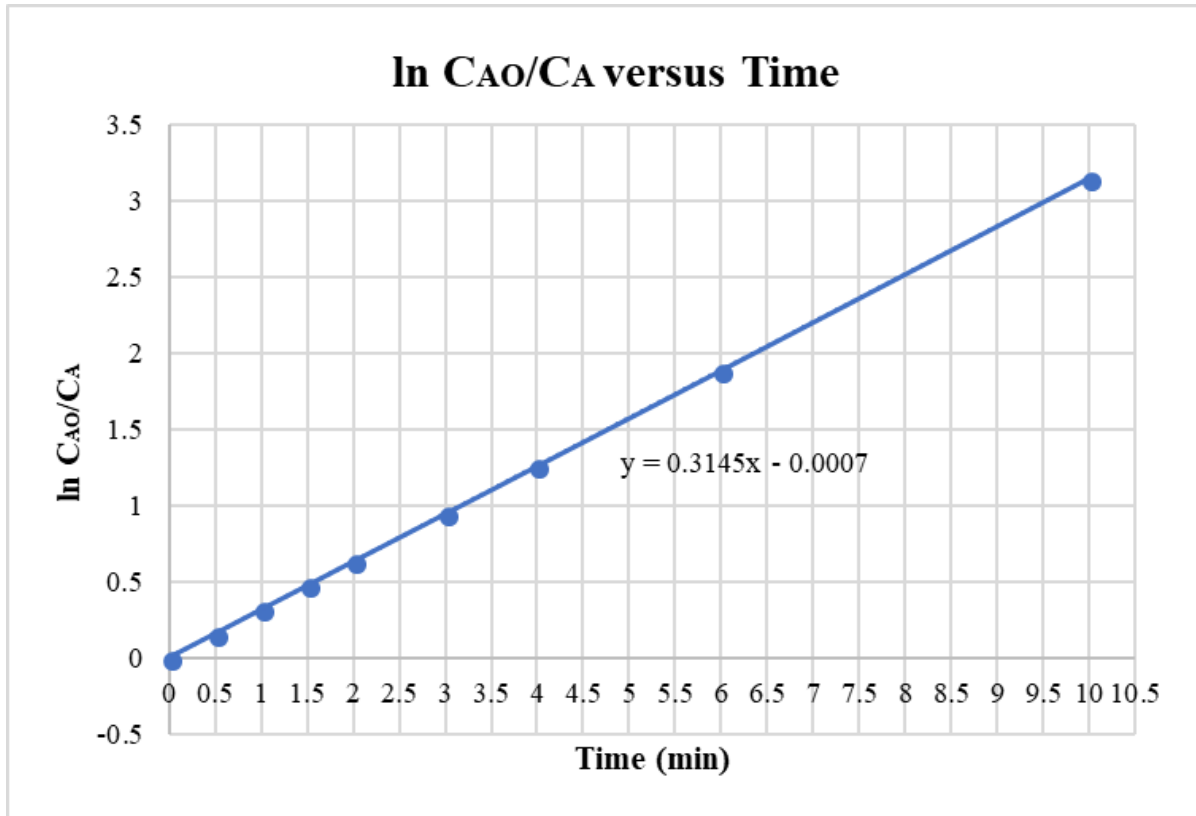$$\int_{C_{AO}}^{C_A} \frac{-dC_A}{C_A} = \int_0^t kdt$$

$$\ln C_{AO} - \ln C_A = kt$$

$$\ln \frac{C_{Ao}}{C_A} = kt$$

$$\ln \frac{C_{Ao}}{C_{Ao} - C_C} = kt$$

The graph of ln (C_{AO}/C_A) against time is plotted to find the rate constant, k at temperature 85°C. From the graph in figure below, the gradient is equal to the rate constant, k.

Figure 4 - Graph of ln CAO/CA against Time

Thus, the slope of the graph, k (358K) = 0.3145/min.

For the inlet feed temperature, our team decided to set the inlet feed temperature to the reactor as T_o = 55°C. Therefore, the rate constant, k at T_o = 55°C =328K is calculated by using Arrhenius Law,

Given:

    i.   Activation energy = 39500 J/mol

    ii.   R=8.314J/mol.K

$$k = Ae^{-E/RT}$$

$$k(T) = k_o(T)\exp\left[\frac{E}{R}\left(\frac{1}{T_O} - \frac{1}{T}\right)\right]$$

$$k(328K) = 0.3145\text{min}^{-1}\exp\left[\frac{39500J/mol}{8.314J/mol.\,K}\left(\frac{1}{358K} - \frac{1}{328K}\right)\right]$$

$$k(328K) = 0.0934\text{min}^{-1}$$

Design Reactor for CSTR

$$V = \frac{F_{AO}X}{-r_A}$$

$$V = \frac{F_{AO}X}{kC_A}$$

Information given,

i. Conversion, $X = 0.8$

ii. Volume = 1000L

iii. Inlet feed temperature, $T_o = 55^{\circ}C = 328K$

iv. Activation energy = 39500 J/mol

v. R=8.314J/mol.K

vi. $C_{AO} = 16$kmol/L

vii. $F_{AO} = 1600$kmol/L

viii. $F_{BO} = 3200$kmol/L

1) The total volumetric flowrate, v_o

a) The volumetric flowrate of ethylene oxide is half of the volumetric flowrate of water.

$$v_{Ao} = \frac{1}{2}v_{Bo}$$

b) The volumetric flowrate of ethylene oxide, v_{AO}

$$F_{AO} = C_{AO}v_{Ao}$$

$$v_{Ao} = \frac{F_{AO}}{C_{A0}}$$

$$v_{Ao} = \frac{1600\text{kmol/min}}{16\text{kmol/L}}$$

$$v_{Ao} = 100\text{L/min}$$

c) The volumetric flowrate of water, v_{BO}

$$v_{Bo} = 2v_{Ao}$$

$$v_{Bo} = 2(100\text{L/min})$$

$$v_{Bo} = 200\text{L/min}$$

d) The total volumetric flowrate, v_o

$$v_o = v_{AO} + v_{BO}$$

$$v_o = (100 + 200)\text{L/min}$$

$$v_o = 300\text{L/min}$$

2) Space time, τ

$$\tau = \frac{V}{v_o}$$

$$\tau = \frac{1000L}{300L/min}$$

$$\tau = 3.3333 min$$

3) Mole Balance Conversion, X_{MB}

From rate constant, k_o (328K)=0.0934min^{-1}, calculate the rate constant, k at temperature range from 298K to 473K, in order to calculate the X_{MB}.

For example: T=298K

$$k(298K) = 0.0934 min^{-1} exp\left[\frac{39500J/mol}{8.314J/mol.K}\left(\frac{1}{328K} - \frac{1}{298K}\right)\right]$$

$$k(298K) = 0.0217 min^{-1}$$

$$X_{MB} = \frac{\tau Ae^{-E/RT}}{1 + \tau Ae^{-E/RT}}$$

$$X_{MB} = \frac{\tau k}{1 + \tau k}$$

$$X_{MB} = \frac{3.3333 min(0.0217 min^{-1})}{1 + 3.3333 min(0.0217 min^{-1})}$$

$$X_{MB} = 0.0676$$

4) Heat of Reaction, $\Delta \hat{H}_{RX}^o$ using Heat of Formation Method at T_{ref}

$$\Delta H_i^o(T) = \Delta \hat{H}_{f.i}$$

$$\Delta H_A^o(298K) = -26.3 \text{ kJ/mol}$$

$$\Delta H_B^o(298K) = -142.7 \text{ kJ/mol}$$

$$\Delta H_C^o(298K) = -193.5 \text{ kJ/mol}$$

$$\Delta \hat{H}_{RX}^o(T) = \sum_{product} |v_i|\Delta \hat{H}_{f.i} - \sum_{Reactant} |v_i|\Delta \hat{H}_{f.i}$$

$$\Delta \hat{H}_{RX}^o(298K) = (1)(-193.5) - \big((1)(-26.3) + (1)(-142.7)\big) \text{ kJ/mol}$$

$$\Delta \hat{H}_{RX}^o(298K) = -24.5 \text{ kJ/mol}$$

$$\Delta \hat{H}_{RX}^o(298K) = -24\,500 \text{ J/mol}$$

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5) Heat Capacity of The Component, Cp_i

a) Ethylene Oxide (A)

$$Cp_A(T) = 7.52 + 0.2222T + 1.256 \times 10^{-4}T^2 + 2.592 \times 10^{-8}T^3$$

$$Cp_A(328K) = 7.52 + 0.2222(328K) + 1.256 \times 10^{-4}(328K)^2 + 2.592 \times 10^{-8}(328K)^3$$

$$Cp_A(328K) = 94.8288 \text{ J/mol}$$

b) Water (B)

$$Cp_B(T) = 13.823 + 0.0104T$$

$$Cp_B(328K) = 13.823 + 0.0104(328K)$$

$$Cp_B(328K) = 17.2342 \text{ J/mol}$$

c) Ethylene Glycol (C)

$$Cp_B(T) = 78 \text{ J/mol}$$

6) ΔCp

$$\Delta Cp = Cp_C - Cp_B - Cp_A$$

$$\Delta Cp = 78 \text{ J/mol} - 17.2342 \text{ J/mol} - 94.8288 \text{ J/mol}$$

$$\Delta Cp = -34.0630 \text{ kJ/mol}$$

7) Θ_i

$$\Theta_A = \frac{F_{AO}}{F_{AO}} = \frac{1600 \text{ kmol/min}}{1600 \text{ kmol/min}} = 1$$

$$\Theta_B = \frac{F_{BO}}{F_{AO}} = \frac{3200 \text{ kmol/min}}{1600 \text{ kmol/min}} = 2$$

$$\Theta_C = \frac{F_{CO}}{F_{AO}} = \frac{0 \text{ kmol/min}}{1600 \text{ kmol/min}} = 0$$

8) $\sum \Theta_i Cp_i$

$$\sum \Theta_i Cp_i = \Theta_A Cp_A + \Theta_B Cp_B$$

$$\sum \Theta_i Cp_i = (1)(94.8288 \text{J/mol}) + (2)(17.2342 \text{ J/mol})$$

$$\sum \Theta_i Cp_i = 129.2972 \text{ J/mol}$$

9) Conversion Calculated From Energy Balance, X_{EB}

$$X_{EB} = \frac{\Sigma \theta_i C_{pi}(T - T_O)}{-\Delta H_{RX}^\circ(T_R) + \Delta C_p(T - T_R)}$$

At T = 328 K

$$X_{EB} = \frac{(129.2972 \text{ J/mol. K})(328 \text{ K} - 328 \text{ K})}{-(-24500 \text{ J/mol}) + (-34.0630 \text{ J/mol. K})(328 \text{ K} - 298 \text{ K})}$$

$$X_{EB} = 0.0000$$

Table 2 – The Calculated Conversion from Material Balance and Energy Balance

Temperature		Material Balance		Energy Balance
T(°C)	T (K)	k (min⁻¹)	X_{MB}	X_{EB}
55	328	0.0934	0.2375	0.0000
57	330	0.1020	0.2537	0.0110
75	348	0.2148	0.4172	0.1134
100	373	0.5363	0.6413	0.2651
125	398	1.1936	0.7991	0.4291
150	423	2.4170	0.8896	0.6068
175	448	4.5235	0.9378	0.8002
200	473	7.9232	0.9635	1.0113
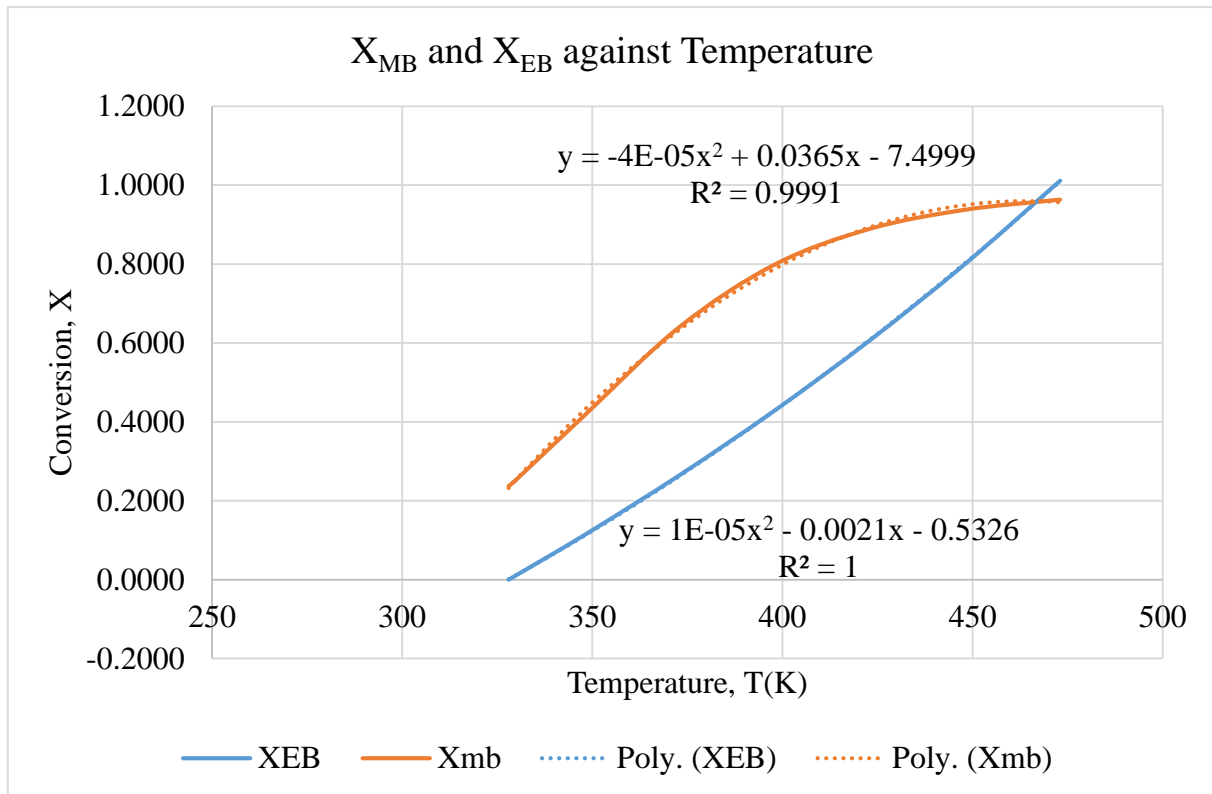
Figure 5 - Graph of Conversion Calculated From Material Balance, X_{MB} and Conversion Calculated From Energy Balance, X_{EB} against Temperature, T

Based on the plotted graph, the intersection between the X_{EB} and X_{MB} line represent the equilibrium conversion at equilibrium temperature for the reaction. Thus, the equilibrium conversion, $X_E = 0.96$ at equilibrium temperature of $T_E = 470$ K = 197°C. Based on the equilibrium data obtained, the reactor can be used to replace the leaked reactor. Since, the reaction is carried out at constant temperature of 85°C and it did not exceed the reactor limit which is 125°C.

However, the reaction will only reached equilibrium at 197°C. Thus, although the reactor can be used, it is impossible for the reaction to reached equilibrium if 55°C is set to be the initial temperature of feed into the reactor. It is vital to re-assess the reactor feasibility using different initial temperature. Unable to reach equilibrium will resulting in inconsistency of reactants and products concentration with time. Thus, affecting in the output ethylene glycol to be obtained. Besides, in case of the reaction reached equilibrium, the replaced reactor will face the same problem as the previous reactor since the reactor cannot handle the equilibrium temperature. Problems like leaking or exploding could occur due to this problem.

There are few ways to increase the conversion of ethylene oxide to ethylene glycol. Firstly, we can increase the concentration of the ethylene oxide used. By increasing the amount of reactants, the rate of reaction will also increases since the high concentration of reactants will lead to more effective collisions per unit time. This will lead to an increased reaction rate except for the water which is in excess and is apparently zero-order. Besides, the temperature of the reaction can be increases. This will also increase the rate of reaction between ethylene oxide and water. Other than that, we can also use catalyst such as amine compounds, bi-functional compounds and Salen compounds. The way catalyst works is by increasing the frequency of collisions between ethylene oxides and water so that more effective collisions is happening. Thus, increases the rate of the reaction and lower the activation energy of the chemical reaction.

4.0   DETAIL DESIGN

Assumption:

   i.   Steady State; $\frac{dN_A}{dt} = 0$

   ii.   Well mixed;

$$\int_0^V r_A dV = r_A \int_0^V dV = r_A V$$

1. Mole Balance and Design Equation

$$F_{AO} - F_A + r_A V = 0 \qquad \textbf{Equation 1}$$

Design Equation for CSTR

$$V = \frac{F_{AO} - F_A}{-r_A} = \frac{F_{AO}X}{-r_A} \qquad \textbf{Equation 2}$$

2. Rate Law

Since the reaction is first order;

$$-r_A = kC_A \qquad \textbf{Equation 3}$$

3. Stoichiometry (liquid phase, v=vo):

$$C_A = C_{AO}(1 - X) \qquad \textbf{Equation 4}$$

4. Combining yields (from equation 2,3 and 4)

$$V = \frac{F_{AO}X}{kC_{AO}(1-X)} = \frac{C_{AO}v_O X}{kC_{AO}(1-X)} = \frac{v_O X}{k(1-X)} \qquad \textbf{Equation 5}$$

Solving for X as a function of T whereby **τ= V/ vo**

$$X_{MB} = \frac{\tau k}{1 + \tau k} = \frac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}} \qquad \textbf{Equation 6}$$

This equation is form by the relation of temperature and conversion through mole balance.

5. Energy Balance

Since the reaction is adiabatic, energy input is negligible. Thus,

$$X_{EB} = \frac{\Sigma\theta_i C_{pi}(T - T_O)}{-\Delta H^{\circ}_{RX}(T_R) + \Delta C_p(T - T_R)} \qquad \textbf{Equation 7}$$

5.0 SAFETY FACTOR

5.1 EXPOSURE POTENTIAL

Based on the uses for ethylene glycol, the public could be exposed through:

5.1.1 Workplace Exposure

The use of enclosed equipment, engineering controls, and personal protective equipment during the manufacture of ethylene glycol minimize the potential for human exposure. The most likely route of exposure is industrial, either in ethylene glycol production facilities using products containing ethylene glycol. Those working with ethylene glycol could be exposed during maintenance, sampling, testing, or other procedures. Each manufacturing facility should have a thorough training program for employees about appropriate work processes and safety equipment in place to limit unnecessary chemical exposure.

5.1.2 Consumer Exposure To Products Containing Ethylene Glycol

Consumers could come into contact with ethylene glycol rarely and only for short periods for example, when adding antifreeze/coolant to vehicles. Consumers may also be exposed to small amounts of ethylene glycol.

5.1.3 Environmental Releases

Ethylene glycol production or the use of ethylene glycol or products containing ethylene glycol could result in the release of this material to the environment through various waste streams. In the event of a spill, the focus is on containing the spill to prevent contamination of soil and surface or ground water. For small spills, contain the material if possible. Absorb with materials such as cat litter, sand, or sawdust. Collect in suitable and properly labelled containers and dispose of this material in compliance with all governmental requirements.

5.1.4 Large Release

For large spills, dike the area. Pump the recovered material into suitable and properly labelled containers and dispose in compliance with all governmental requirements. Keep unnecessary personnel and wildlife from entering area. Use

appropriate safety equipment. Follow emergency procedures carefully. In case of fire, use water fog, fine water spray, or dry-chemical or carbon dioxide fire extinguishers to extinguish the fire. Burning liquids may be extinguished by dilution with water, but do not use a direct water stream. During a fire, smoke may contain the original material in addition to toxic or irritating combustion products. Fight fire from a protected location or safe distance. Consider the use of unmanned hose holders. Fire-fighters should wear positive-pressure, self-contained breathing apparatus (SCBA) and protective fire-fighting clothing.

5.2   HEALTH

Eye contact with the liquid, vapour, or mist may cause slight irritation. Corneal injury is unlikely. Brief contact is essentially no irritating to skin. Prolonged or repeated contact may cause slight skin irritation with local redness. Repeated skin exposure to large quantities of ethylene glycol may result in absorption of harmful amounts. Massive contact with damaged skin or with material hot enough to burn the skin may result in absorption of potentially lethal amounts. At room temperature, exposure to vapour is minimal due to its low volatility. With good ventilation, a single exposure is not expected to cause adverse effects. If the material is heated or areas are poorly ventilated, vapour or mist may accumulate and cause respiratory irritation and symptoms such as headache and nausea.

The oral toxicity of ethylene glycol is moderate. Small amounts swallowed incidentally as a result of normal handling operations are not likely to cause injury; however, swallowing large amounts of ethylene glycol may cause nausea, vomiting, abdominal effects, diarrhea, and/or serious injury-even death. Excessive exposure may result in central nervous system effects, cardiopulmonary effects, and kidney failure. Repeated excessive exposure may cause irritation of the upper respiratory tract. In humans, effects have been reported on the central nervous system. In animals, effects have been reported on the kidney and liver.

Ethylene glycol did not cause cancer in long-term animal studies. Based on animal studies, ingestion of very large amounts of ethylene glycol appears to be the major and possibly only route of exposure to produce birth defects. Ingested in large amounts, ethylene glycol has also been shown to interfere with reproduction in animals. In vitro and animal genetic toxicity studies were negative.

5.3 ENVIRONMENTAL

Ethylene glycol is practically nontoxic to aquatic organisms on an acute basis. Ethylene glycol is readily biodegradable, its bio concentration (accumulation in the food chain) potential is low, and its potential for mobility in soil is very high. However due to the fact that Ethylene Glycol is readily biodegradable in water and will consume oxygen in this process it could cause a depletion of oxygen in bodies of water that could harm aquatic organism. Ethylene glycol is thermally stable at recommended storage and use temperatures and pressures. Exposure to elevated temperatures can cause decomposition. Gas generated during decomposition can cause pressure build-up in closed systems. The decomposition products of ethylene glycol depend upon temperature, air supply, and the presence of other materials and may include aldehydes, alcohols, and ethers. Ethylene glycol is incompatible with strong acids, strong bases, and strong oxidizers. Avoid contact with these materials. Spills of ethylene glycol on hot fibrous insulation may lead to a reduction of the auto ignition temperature, resulting in the potential for spontaneous combustion.

6.0   REFERENCES

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7.0   APPENDICES

Table 3 - Additional Information Provided in Assignment Question

Chemical species	Heat of formation at 25°C (kJ/mol)	Heat Capacity (J/mol.K) : $C_p = a + bT + cT^2 + dT^3$			
		a	b	c	d
Ethylene oxide	-26.3	7.52	0.2222	1.256×10^{-4}	2.592×10^{-8}
Water	-142.7	13.823	0.0104		
Ethylene glycol	-193.5	78.00			

Activation Energy: 39,500 J/mol

Table 4 - Material Balance Data to Calculate For Conversion, X_{MB}

Time (min)	Cc	Cao	Cao/ (Cao-Cc)	ln (Cao/ (Cao-Cc))	k_o (T=85)	k_o (T=55)	τ	E	R	T_o (K)	T (K)	k	X_{MB}
0	0.0000	1	1.0000	0.0000	0.3145	0.0934	3.3333	39500	8.314	328	328	0.0934	0.2375
0.5	0.1450	1	1.1696	0.1567	0.3145	0.0934	3.3333	39500	8.314	328	330	0.1020	0.2537
1	0.2700	1	1.3699	0.3147	0.3145	0.0934	3.3333	39500	8.314	328	348	0.2148	0.4172
1.5	0.3760	1	1.6026	0.4716	0.3145	0.0934	3.3333	39500	8.314	328	373	0.5363	0.6413
2	0.4670	1	1.8762	0.6292	0.3145	0.0934	3.3333	39500	8.314	328	398	1.1936	0.7991
3	0.6100	1	2.5641	0.9416	0.3145	0.0934	3.3333	39500	8.314	328	423	2.4170	0.8896
4	0.7150	1	3.5088	1.2553	0.3145	0.0934	3.3333	39500	8.314	328	448	4.5235	0.9378
6	0.8480	1	6.5789	1.8839	0.3145	0.0934	3.3333	39500	8.314	328	473	7.9232	0.9635