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Research Article

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Design of a Plant for the Production of 350,000tone/Yr of Ethylene Oxide Using Ethylene and Oxygen

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ABSTRACT

The manual design of 350kt/yr ethylene oxide production plant from ethylene oxy-catalytic process has been developed. The essential units of the ethylene oxide plant that the design followed were catalytic packed reactor, packed column and Distillation column. The design process conditions for ethylene oxide production are 130-150 °C, 1 atm and metal-oxide Ag-catalyst at conversion rate of 0.9. The following results were obtained; Volume of reactor 372.74 m^3 , Diameter of 3.20 m and 3.24 m respectively for packed column and Distillation column gave overall height of 6.48 m and 17.2 m respectively for Distillation column and packed column. Further the manual design was validated with the HYSYS design simulation.

Key words: Manual Design, Ethylene Oxide, Oxy-catalytic Process, Conversion Rate and Production Process

1. INTRODUCTION

Ethylene oxide (EO) is a basic chemical produced primarily by the catalytic oxidation of ethylene. It is a chemical intermediate that cannot be directly used and is further reacted to produce a wide spectrum of products. Ethylene glycols (mono-, di-, triethylene glycol) constitute by far the single-largest outlet for ethylene oxide, accounting for about 65% of the EO market in 2018 [1]. Other dominant end uses include higher-value derivatives such as ethoxylates, ethanolamines, glycol ethers, polyethylene glycol, and polyether polyols.



Fig. 1 Pie chart shows world consumption of ethylene oxide [1, 2]

As of 2018, EO was produced primarily in Northeast Asia, the Middle East, and North America, accounting for a combined 77% of global production. In these three regions, a significant portion of the producers are forward-integrated into the production of MEG and the EO consumption pattern is therefore broadly similar to the MEG production footprint globally.

The Middle East was quite active between 2005 and 2010, with new EO capacity additions. The region was capitalizing on the availability of extremely cheap ethane to competitively produce ethylene and downstream ethylene derivatives, including ethylene oxide. But the pace of new additions in the Middle East has slowed with a clear shift in new capacity

going to North America. Between the late 1990s and the late 2000s, North America lost significant momentum on the back of new large-scale EO capacity commissioning in the Middle East and Northeast Asia [2]. In the United States, EO/EG producers had lost their competitive edge because of higher raw material costs and aging production units. Over the last decade, the net EO capacity change was therefore negative in North America. The advent of shale gas production in the region has changed the state of the US and North American petrochemical industry. Natural gas liquids coproduced along with natural gas (ethane and propane, essentially) are now competitively priced feedstock readily available to the petrochemical industry. As a result, the new petrochemical project pipeline has significantly picked up in North America and new EO capacity will be started up through 2023.

Overall demand for ethylene oxide is tied to the general economy and has been increasingly linked to emerging countries, where the improvement in living standards is driving an increasing usage of a broad spectrum of polymers and chemicals that are further used for the production of packaging, films, textile fibers, soaps, detergents, etc. Over the coming five years, overall demand for ethylene oxide is expected to increase further, fueled primarily by an incremental demand for polyester products, antifreeze, polyurethanes, soaps, detergents, etc. in emerging regions [2, 3].

Like all other petrochemicals, the ethylene oxide industry is cyclical, with the equilibrium between supply and demand driving the state of the industry. In times of large concomitant new capacity commissioning, operating rates generally go down and margins contract because of increased competition among producers. As margins remain under pressure, no new capacity is built (trough conditions) [3]. When demand gradually catches up with production, operating rates firm up and margins expand. This is when the next wave of capacity is generally planned (and the next cycle begins). Peak conditions were prominent within the ethylene oxide industry between 2011 and 2015, but the ethylene oxide industry is currently facing five years of forecast oversupply, which will inevitably put pressure on operating rates. These conditions will be related to new capacity increasing faster than demand. The slowdown in EO demand growth will also further exacerbate the supply glut seen in the industry.

The Physical Properties of ethylene oxide are as follows [4]:

Chemical formula for ethyleneoxide is C_2H_4O , and the molecular weight is 44.1 g/mol; vapour pressure for ethyleneoxide is 1.095mmHg at 20 °C, and it has an octanol/water partition coefficient; (log[Kow]) of -0.22; Ethyleneoxide has solubility in water of 1×10^6 mg/L at 20 °C and is soluble in alcohol, ether, acetone, and benzene; Ethyleneoxide has an odor threshold of 787 mg/m³ and Ethylene oxide has an estimated half-life in air ranging from 69 to 149 days, while its half-life in water ranges from 12 to 14 days in sterile, deionized, and natural river water.

The important of the product Ethylene Oxide as a petrochemical raw materials and also essential chemical in the petrochemical plant and chemical industries lead to this design [2].

Various authors talked about the production of ethylene oxide by: Person, (2015) [5] researched on the simulation model of a reactor for Ethylene oxide production, where Aspen plus was used to create a simulation model that correlate with reality. John, et al., (2008) [6], briefed on the importance of Ethylene oxide as raw materials in the chemical and petrochemical plant

Process Analyzers in Ethylene oxide production plant was established by oil and gas industry (Siemens) June 2003. This industry considers the packed bed catalytic reactor for production of Ethylene oxide from oxygen and ethylene and the instrumentation processes of the full plant.

Bteon, et al., (2002) [7] researched on the design ethylene oxide purification system in which ethylene oxide is produced by partial oxidation of ethylene. 99.95% purity goal was achieved for this work.

The project aimed at designing 350,000 tons/yr of Ethylene oxide plant from catalytic reaction of ethylene and oxygen. To achieve this aim, the following steps are noted for the design: study the feasibility of the plant possibility of the design set-up for the production of 350,000 tone/yr of Ethylene Oxide; Hysys simulation of the 350kt/yr of Ethylene Oxide; design essential units of the 350,000 tons/yr of Ethylene oxide such as Reactor, Distillation and Packed column; to do the mechanical design of these units and cost the units in dollars and to consider the plant layout and instrumentation control and safety, hazards and environmental consideration.

Process Description



To Ethylene glycol and other products

Production of Ethylene oxide is based on catalytic oxidation of ethylene using Ag-catalyst. As shown above, Ethylene oxide produced from a packed bed reactor where ethylene reacts with purification chamber where H_20 is added and ethylene is recycled but the liquid mixture consists of ethylene oxide and ethylene glycol enters the stripping section and overhead product is ethylene oxide collected.

Meanwhile the other gases ethylene, oxygen, N_2 , CO_2 enters the vent column where O_2 and Ethylene are recycled reactor for reaction continuation. The process conditions are as follows;

Process conditions are Temperature 130-150 °C; Pressure 1-3 atm and Flow rate: 350,000 tons/yr

2. MATERIAL BALANCE

Rate of inflow – Rate of outflow + Rate of production = 0 $CH_2 = CH_2 + \frac{1}{2}O_2$ \longrightarrow CH_2 -O- CH_2

$$(r_{EO}) = KC_{\varepsilon} = k(t) P_T y_{e}$$

Kinetic study: LQiang, et al, (2011) [8]

$$k(t) = 9.3 \times 10^{-4} \pm 7 \times 10^{-5} min$$

$$F_A = 0.3069 kmol/s$$

$$y_F = 1 - F_A$$

$$(r_{EO}) = k(t) P_T (1 - X_A) = 0.001 \times 0.9 = 9.0 \times 10^{-4} mol/min = 1.5 \times 10^{-5} mol/s$$

$$V_{PBR} = \frac{F_{AO}}{C_{AO} k(t)} In \left[\frac{1}{1 - X_A}\right]$$

$$V_{PBR} = \frac{0.4603 ln \left[\frac{1}{0.1}\right]}{284.35 \times 1.0 \times 10^{-5}} = 372.74 m^3$$

Material Balance for the packed column

The scrubber is majorly called Ethylene oxide scrubber where gases such as Ethylene oxide, (1-2%); CO₂ (5%) and others such as N₂, CH₂=CH₂, CH₄ and aldehyde after being cooled enters the absorption column where absorbent (H₂O) is used to absorbed the EO alongside CO₂N₂ CH₄= CH₂ and CH₄ [9].



 $G_M = \frac{Fig. 3 \text{ Sketch of Scrubber}}{300 x 24 x 3600} = 0.3069 \text{mol/s}$

$$y_2 = 0.02 \ x \ 0.8 = 0.0016 mol$$

The material balance is given as:

$$G_M y_1 + L_m x^2 = G_M y_2 + L_m x X_1$$
$$L_m = \frac{G_M (y_1 - y_2)}{x_1} = \frac{G_M (98\% y_1)}{x_1}$$
$$= \frac{0.3069 x (0.0784)}{0.00619} = 3.89 kmol/s$$

Thus: $G'_m = 8.9051 kg/s, L'_m = 70.02 kg/s$

$$m = {y_1}/{x_1} = \frac{0.08}{6.19 \times 10^{-3}} = 13$$
$$mG_m/L_m = \frac{13 \times 0.3069}{3.89} = 1.0256$$
$$N_{oG} : {y_1}/{x_2} = {y_1}/{2\% y_1} = 50: N_{oG} = 10.5$$

Material Balance for Distillation Column

Water and EO (Ethylene oxide) are passed into the stripping/Distillation column for the removal of EO as overhead product.

Using Antoine equation parameters

.

 $log_{10}^{(P^*)} = A - [B/(T+C)] [10]$

	= 5.84	696 = [2022.83/T + 62]	.656)]	
		T = 150 + 273		
T °C	P_A^*	v _ P	$T - P_B^* = P_A^* X_A$	
		$\Lambda_A - \overline{P}$	$\frac{f_{A}}{f_{A}} - P_{B}^{*}$ $y_{A} - P_{T}$	
100	15.987	0.1	0.20	
105	18.049	0.2	0.40	
110	20.322	0.3	0.45	
115	22.821	0.4	0.56	
120	25.561	0.5	0.70	
125	28.560	0.6	0.80	
130	31.836	0.7	0.85	
135	35.405	0.8	0.90	
140	39.297	1.0	0.98	
150	48.063			
F=kmo l/s =0.36 X _w =0.64	V R=1.58 V m Lm	→ D = 0.3069kmol $y_D=0.95$ $y_w=0.05$ →B $x'_f=5\%$ w/w $x'_{w}=0.995$	/s	

It is required that 0.31kmol/s was distilled out at 95% mol/mol of Ethylene oxide at the top and 99.55% mol/mol of water was found at the bottom of which 36% mol/mol Ethylene oxide enter the column optimally, Input = output. Total mass balance:

F = D + BF - D = B

Species/components balance:

$$E0:$$

$$x_{f}F = y_{D}D + y_{w}B$$

$$x_{f}F = y_{D}D + y_{w}B(F - D)$$

$$0.36F = 0.95 (0.3069) + 0.05 (F - 0.3069)$$

$$(0.36 - 0.05)F = 0.95 (0.3069) - 0.05 (0.3069)$$

$$0.31F = 0.27621$$

$$F = \frac{0.27621}{0.31} = 0.891 \text{ kmol/s}$$

$$B = F - D$$

$$B = 0.891 - 0.3069 = 0.5841 \text{ kmol/s}$$

$$V_{n} = \frac{L_{n}}{D} \Longrightarrow L_{n} = RD = 0.3069x \ 1.58 = 0.4849 \text{ kmol/s}$$

$$V_{n} = L_{n} + D = 0.4849 + 0.3069 = 0.7918 \text{ kmol/s}$$

$$I_{m} = L_{n} + qf = 0.4849 + 0.7483 = 1.2332 \text{ kmol/s}$$

 $V_n = L_m - B = 1.2332 - 0.5841 = 0.6491 \, kmol/s$

3. ENERGY BALANCE

Energy across the Reactor [9]

From the material balance: $F_{\varepsilon,o} = 0.3069$ kmol/s $F_{o,o} = 0.1535$ kmol/s $F_{\varepsilon,o} = 0.3069$ kmol/s Reactants directed = $(F_{\epsilon,o} + F_{o,o}) - F_{\epsilon,o} = 0.4604 - (0.3069) = 0.1535$ kmol/s Balance: $H_1 + H_2 + Q = \alpha \Delta H_R + H_3$

Where
$$\alpha$$
 = Extent of the reaction = 0.85
Fake T ref = 30 °C = 303k



Fig. 4 Energy balance in catalytic packed bed reactor [11] $\Delta H_R = -13. OKJ/mol$ = -13.0KJ/mol x 0.3069kmol/s x 0.85 = -3.3912KJ/s $H_3 = FCp\Delta T + m \succ_{\varepsilon o} = F(Cp\Delta T + \succ_{\varepsilon o})$ = 0.3069 (0.0479(473 - 303) + 0.0008) = 2.49933KJ/s = 2.5KJ/s $H_1 = F_{\varepsilon o} Cp\Delta T$ = 0.3069 (0.0300 x (120 - 100)) = 0.18414KJ/s $H_2 = 0.1535 x 0.001 x 20 = 0.00307KJ/s$ $(F_{o,o} Cp_{0.2}\Delta T)$ Q = (-3.3912 + 2.5) - (0.00307 + 0.1535) = -1.0478KJ/s

Energy balance across the Distillation column [9] From the material balance:

$$F = 0.891 kmol/s$$

$$D = 0.3069 kmol/s$$

$$B = 0.5841 kmol/s$$

$$L_n = 0.4849 kmol/s$$

$$L_m = 1.2332 kmol/s$$

$$V_m = 0.7918 kmol/s$$



Fig. 5 Energy balance across the Distillation column [9] $Q_B = H_F + H_D - (Q_c + H_B)$ $H_F = FCp_{av}\Delta T$ $Cp_{av} = 0.36Cp_{\varepsilon} + 0.64Cp_w = 0.36 \ x \ 0.030 + 0.64 \ x \ 4.2/18$ = 0.160KJ/kmolk $\Delta T = 20$ $H_F = 0.891 \ (0.160)x \ 20 = 2.8512KJ/s$

$$\begin{split} H_D &= \Delta C p_{av} \Delta T = 0.3069 \ x \ 0.009 \ x \ 170 = 0.4696 \ KJ/s \\ H_B &= B C p_{av} \Delta T \\ &= 0.5841 \ kmol/s \ x \ 0.160 \ x \ 200 \ = \ 18.6912 \ KJ/s \\ Q_c &= V_n \times_{av} \\ \times_{av} &= y_D \times_{\varepsilon 0} + y_w \times_w \\ &= 0.95 \ (0.001) + \ 0.05 \ x \ 2256/18 \ = \ 6.268 \ KJ/mol \\ Q_c &= 0.633 \ kmol/s \ x \ 6.268 \ KJ/kmol \ = \ 3.96 \ KJ/s \\ Q_B &= H_F + H_D - Q_c - H_B \\ Q_B &= (2.85 + 0.4696) - (3.967 + 18.6912) \\ &= (2.3804 - 22.6582) \ = -20.2778 \ KJ/s \end{split}$$

4. EQUIPMENT SIZING AND SPECIFICATION

Sizing of the Reactor [9]

The Diameter and the length of the reactor is determined in other to size and specify the reactor from the material balance.

L = 2.5D

The volume of the reactor = 372.74m³ But L/D = 2.5 [12]

Also,
$$V_{PBR} = \frac{\pi D^2}{4} L$$

$$= \frac{\pi D^2}{4} x \ 2.5D = \frac{\pi D^2}{4} x \ 0.625 \ xD = 0.625 \pi D^3$$

$$\therefore D = \left[\frac{V_{PBR}}{0.625 \pi}\right]^{1/3}$$

$$D = \left[\frac{372.74}{0.625 \pi}\right]^{1/3} = [189.81]^{1/3} = 5.75m$$

L = 2.5D = 2.5 x 4.84 = 14.375 m

Sizing and specification of the packed column [9]

Determining of the packed column diameter unit, the overall height, helps to size and specify the column for absorption process.

From the material balance:

$$G_{m} = 0.3069kmol/s$$

$$L_{m} = 3.89kmol/s$$

$$mG_{m}/L_{m} = 1.0256$$

$$X_{i} = 6.19 \times 10^{-3}$$

$$y_{i} = 0.08$$

$$y_{2} = 0.0016$$

$$F_{p} = 170m^{-1}$$

Column diameter determination

38-min ceramic interlox[®] saddles ρ_g at 30[°]c = $\frac{M_{\epsilon o}}{22.4} x \frac{(273)}{303}$

$$= \frac{44}{22.4} x273/303 = 1.770 kg/m^{3}$$

$$L = 1000 kg/m^{3}$$

$$\mu_{L} = 0.058 Ns/m^{2}$$

$$FL_{V} = \frac{L_{m}}{G_{m}} \sqrt{\frac{\rho_{g}}{\rho_{i}}}$$

$$= \frac{3.89}{0.3069} \sqrt{\frac{1.770}{1000}}$$

$$= \frac{0.1637}{0.3069} = 0.533$$

$$K_{4} = 0.58$$

$$V_{w} = \left[\frac{k_{\rho}\rho_{g}(\rho_{2}-\rho_{g})}{13.1F_{\rho}(\frac{\mu_{L}}{\rho_{L}})}\right]^{1/2}$$

$$\begin{split} &= \left[\frac{0.58 \times 1.770 \ (1000 - 1.1770)}{13.1 \times 170 \ (\frac{0.058}{1000}^{0.1})}\right]^{1/2} \\ &= (1.22)^{1/2} - 1.105kg/sm^2 \\ a_e = \frac{6\pi}{7} k_e^* = \frac{6.99}{6.89} = 3.05m^2 \\ D_e &= (4 \times ac/n)^{1/2} \\ a_w &= a \left[1 - \exp(-1.45 \ (^{-6}/a_L)^{0.25} \ (\frac{10}{a_{LL}})^{0.2} \ (\frac{10}{P_L}^{1/2})^{-0.05} \ (\frac{L_1^{1/2}}{P_L})^{0.2} \right] \\ a &= 194m^2/m^3 \\ a_w &= a \left[1 - \exp(-1.45 \ (^{-6}/a_L)^{0.25} \ (\frac{19.54}{194 \times 0.058})^{0.1} \ (\frac{19.54 \times 194}{10^{\circ}9.811})^{-0.05} \right] \\ \left[\left(\frac{19.54}{10^{3} \times 70 \times 10^{-3} \times 194}\right)^{0.2} \right] \\ a_w &= 194 \left\{1 - \exp[-1.45 (61/70)^{0.75} \ (\frac{19.54}{194 \times 0.058})^{0.1} \ (\frac{19.54 \times 194}{10^{\circ}9.811})^{-0.05} \right\} \\ \left[\left(\frac{19.54}{10^{3} \times 70 \times 10^{-3} \times 194}\right)^{0.2} \right] \\ a_w &= 194(1 - \exp[-1.45 (0.002) (1.057) \times (1.277) \times (0.4895)) \\ &= 194(1 - \exp[-1.45 (0.003) (1.057) \times (1.277) \times (0.4895)) \\ &= 194(1 - \exp[-1.45 (0.003) (1.057) \times (1.277) \times (0.4895)) \\ &= 194(1 - \exp[-1.65 \times 10^{-5} m/s] \\ k_L (^{0L}/\mu_Lg)^{1/3} &= 0.0051 \ (\frac{112.55}{122.068} \times 10^{-1}) = 194(1 - 0.42) \\ &= 112.25m^2/m^3 \\ k_L (^{0L}/\mu_Lg)^{1/3} &= 0.0051 \ (\frac{112.55}{122.068} \times 10^{-3}) \\ k_E \left(\frac{127.66}{122.068} \times 10^{-5} m/s \\ k_E \left(\frac{127.66}{122.068} \times 10^{-5} m/s \\ k_E \left(\frac{RT}{a_{D_e}}\right)_e = k_E \left(\frac{6}{(A\mu_H)}\right)^{0.7} \ (\frac{100 \times 17 \times 10^{-3}}{100 \times 17 \times 10^{-3}}\right)^{1/3} (194 \times 0.038)^{0.4} \\ k_E \left(\frac{1008314 \times 303}{194 \times 1.45 \times 10^{-5}}\right) = 5.23 \ (\frac{10015}{194 \times 0.018 \times 10^{-3}}\right)^{0.7} \ (\frac{100.888}{10}(18 \times 10^{-2}) \\ k_E \left(\frac{8529}{194 \times 145 \times 10^{-5}}\right) = 5.23 \ (\frac{10015}{194 \times 0.018 \times 10^{-3}}\right)^{0.7} \ (194 \times 0.038)^{-2.0} \\ k_G \left(\frac{4529}{194 \times 112.55 \times 50.55} = 5.23(3)(0.888)(148 \times 10^{-2}) \\ k_G \left(\frac{4529}{194 \times 0.018 \times 10^{-3}}\right)^{0.7} \ (194 \times 0.038)^{-2.0} \\ k_G \left(\frac{4529}{194 \times 112.55 \times 10^{-3}}\right)^{0.7} \ (194 \times 0.038)^{-2.0} \\ k_G \left(\frac{6}{195 \times 10^{-5}} + \frac{1015}{100} = 0.055 \ kmol/sm^2 \\ k_G \left(\frac{6}{1000 \times 10^{-3}} + \frac{1015}{1000 \times 10^{-3}} + \frac{100}{1000 \times 10^{-3}} \right)^{1/3} x (194 \times 0.038)^{-2.0} \\ k_G \left(\frac{6}{1000 \times 10^{-3}} + \frac{100000000000000$$

Equipment sizing and specification of Distillation column [9]

$$\begin{split} \Delta_{P} = Patm + \rho_{gh}x \, No. \, of \, traysPatm \\ = 1.01325 \, bar + 10^{3} \, x \, 9.81 \, x \, 100 \, x \, 10^{-3} \, x \, 12 \, x \, 10^{-5} = 1.131 \, bar \\ \rho_{g}: 1.1 & 1.549 \\ 1.131 & x \\ 1.2 & 1.428 \\ \hline \frac{1.131 - 1.1}{1.2 - 1.1} = \frac{x - 1.549}{1.428 - 1.549} \\ 0.031 \, x \, (1.428 - 1.549) = 0.1 \, (x - 1.549) \\ -0.03751 + 1.549 = x \\ x = 1.51149 \\ \rho_{g} = 1/x = 0.662 \, kg/m^{3} \\ \rho_{L} = 1/v_{f} = 1/0.1003 \, x 10^{-2} = 999.7 \, kg/m^{3} \\ \rho_{\ell}^{\ell} = 882 \, kg/m^{3} \\ \rho_{\ell}^{\nu} = \frac{P}{RT} = \frac{1.131 \, x \, 10^{5}}{8.314 \, x \, (10.4 + 273)} = 48 \, kg/m^{3} \end{split}$$

Column Diameter Determination

Given ΕO water [9] $\begin{array}{l}
\rho_L = 882 \\
\rho_g = 48
\end{array}$ $\rho_L = 999.7$ $\rho_g = 0.662$

F = 0.891 kmol/s
D = 0.3069 kmol/s
B = 0.5841 kmol/s
$L_n = 0.4849 kmol/s$
$L_m = 1.2332 kmol/s$
$V_m = 0.7918 kmol/s$

Operating line calculation UOL:

$$y_n = \frac{L_n}{V_n} x_n + D^{y_D} / V_n$$

= $\frac{0.4849}{0.7918} x_n + \frac{0.95(0.3069)}{0.7918} y_n = 0.61 x_n + 0.37$

LOL:

$$y_m = \frac{L_m}{V_m} x_m - \frac{Bx'_f}{V_m}$$
$$= \frac{1.2332}{0.7918} x_m - \frac{0.5814 \times 0.005}{0.7918}$$
$$y_m = 1.5575 x_m - 0.003671$$

q line:
$$y_q = \left(\frac{q}{1-q}\right)x_q - \frac{x_f}{q-1}$$

 $= \frac{1.05}{0.05} x_q - \frac{0.36}{0.05}$ = 21 x_q - 7.2 m = tanθ $\theta = tan^{-1}(m) = tan^{-1}(21)$ = 87.3⁰ From the given McCabe-Thiele plot, No. of theoretical trays = 7 [9, 13] Assumed Efficiency of the column = 0.6. Actual No. of plates = 7/0.6= 12trays

$$FL_{Vb} = \frac{1.2332}{0.7918} \sqrt{\frac{\rho_v}{\rho_i}}$$
$$= \frac{1.2332}{0.7918} \sqrt{\frac{0.662}{1000}} = 0.04058$$

$$FL_{Vb} = \frac{L_n}{V_n} \sqrt{\frac{\rho_v}{\rho_l}}$$

$$= \frac{0.4849}{0.7918} \sqrt{\frac{48}{882}} = 0.1429$$

$$k_{1b} = 0.095$$

$$k_{1c} = 0.085$$
Correction of $k_1 values$

$$k'_{1b} = k_{1b} (\sigma_u / 0.02)^{0.2}$$

$$= 0.095 x \left(\frac{15}{20}\right)^{0.2} = 0.039688$$

$$k'_{1t} = (\sigma_u / 0.02)^{0.2} k_{1t} = 0.056 \left(\frac{75}{20}\right)^{0.5} = 3.48 m/s$$

$$U_{fb} = k'_{1b} \sqrt{\frac{\rho_c - \rho_g}{\rho_g}} = 0.112$$

$$U_{fb} = k'_{1c} \sqrt{\frac{\rho_c - \rho_g}{\rho_g}} = 0.112 \sqrt{\frac{943.4 - 0.645}{0.662}} = 3.82 m/s$$

$$U_{ft} = k'_{1t} \sqrt{\frac{\rho_c - \rho_g}{\rho_g}} = 0.112 \sqrt{\frac{943.4 - 0.645}{0.646}} = 3.82 m/s$$

$$U_{ft} = k'_{1t} \sqrt{\frac{\rho_c - \rho_g}{\rho_g}} = 0.112 \sqrt{\frac{943.4 - 0.645}{0.646}} = 3.82 m/s$$

$$U_{fb} = 0.85 U_{fb} = 2.958 m/s$$

$$U_{nb} = 0.85 U_{ft} = 0.396 m/s$$

$$U_{nb} = 0.85 U_{ft} = 0.396 m/s$$

$$U_{nb} = 0.85 U_{ft} = 0.396 m/s$$

$$U_{nb} = 0.7258 / 0.3961 = 1.83 m^3/s$$
Column area (Ac)
$$A_{nc} = \frac{a_{nb}}{0.88} = \frac{7.28}{0.38} = 8.27 m^2$$

$$A_{ct} = \frac{A_{nt}}{0.88} = 1.83/0.88 = 2.08 m^2$$
Column diameter (Dc)
$$D_c = \left(\frac{4ac}{\pi}\right)^{1/2}$$

$$D_{c} = \left(\frac{4ac}{\pi}\right)^{1/2}$$
$$D_{cb} = \left(\frac{4x8.27}{\pi}\right)^{1/2} = 3.24m$$
$$D_{ct} = \left(\frac{4x2.08}{\pi}\right)^{1/2} = 1.63m$$

Liquid flow pattern $\hat{V} = \frac{L_m M_B}{\rho_L} = \frac{1.2332 \text{ x } 44}{889.7} = 6.1 \text{ x } 10^{-2}$ Double pass HE needed a diameter of 3.24m.

5. MECHANICAL DESIGN [9]



t = CpDe
$$\sqrt{\frac{Pi}{f}}$$
 + e = 0.4 x 5750 $\sqrt{\frac{0.99}{130}}$ + 2 = 181mm

22.5mm

=

c) Doomed head Ellipsidal head

$$T = \frac{P_1 D_1}{2 f J - 0.2 P_i} + e \qquad = \frac{0.99 \times 5750}{260 - 0.2 * 0.99} + 2 = 22.4 \text{mm}$$

ii. torispherical head

$$t = \frac{P_{i1}D_1C_s}{2fJ + P_1(C_s = 0.2)} + e$$

$$C_s = 1.77$$

$$t = \frac{0.99 \times 5750 \times 1.77}{260 + 0.99(1.77 - 0.2)} + 2mm = 38.4 \text{mm}$$

Hence Ellipsoidal head is acceptable together with the cylindrical shell to make better build0up and reduces cost [9]. **Packed column mechanical design**

Material type: Stainless steel (321) [9] Design pressure, Pi = (5-1) x 0.11 = 0.44 N/mm² Design stress, f - 140N/mm² Design diameter, Di = 3200mm C_p = fully gasket = 0.4 Fully radiographed welds = J=1

 $R_k = 6\% R_c = 6\% D_i$

Corrosion Allowance, e = 1.25mm

$$t = \frac{P_i D_i}{2ft - P_i} + e$$

$$\frac{= 0.44 \times 3200}{280 - 0.44} + 125mm = 7.75mm$$

$$t = C_p D_c \sqrt{\frac{P_i}{f}} + e$$

$$= 0.4 \times 3200 \sqrt{\frac{0.44}{140}} + 125 = 68.4mm$$

(3) Doomed heads

2 Flat head

(I) Ellipsoidal head

$$t = \frac{P_i D_i}{2fJ - 0.2P_i} + e$$
$$= \frac{0.44 \times 3200}{280 - 0.2(0.44)} + 1.25 = 7.75mm$$

(II) Torispherical head

$$t = \frac{P_i R_c C_s}{2fJ + p_i (5 - 0.2)} + e$$

$$\frac{0.44 \ x \ 3200 \ x \ 1.77}{280 + 0.44 (1.77 - 0.2)} + 1.25 = 11.20 mm$$

Cylindrical shell and Ellipsoidal head accepted for the design [9] Packed Column Mechanical Design



Stainless steel (321) Design pressure = $P_i = (10 - 1)x0.11 = 0.99N/mm^2$ Design stress, f = 130N/mm² Design Diameter, D_i = 3240mm (1) Cylindrical shell

$$t = \frac{P_i D_i}{2ft - P_i} + e$$

$$\frac{0.99 \times 3240}{260 - 0.99} + 1.25mm = 12.38mm$$

$$t = 12.38mm$$

(2) Flat ends

$$t = C_p D_c \sqrt{\frac{P_i}{f}} + e$$

 C_p = full face gasket = 0.4

$$D_c = D_i = 3240mm$$
$$t = 0.4 x \ 3240 \sqrt{\frac{0.99}{130}} + 1.25 = 114.34mm$$

(3) Doomed heads

(I) Ellipsoidal head

$$t = \frac{P_i D_i}{2fJ - 0.2P_i} + e$$

(II) Torispherical end

$$\frac{0.99 \times 3240}{260 - 0.2(0.99)} + 1.25$$
$$= \frac{3207.6}{259.802} + 1.25 = 12.38mm$$
$$t = \frac{P_i R_c C_s}{2fJ + p_i (5 - 0.2)} + e$$
$$t = \frac{0.99 \times 3240 \times 1.77}{260 + 0.99(1.77 - 0.2)} + 1.25 = 21.71mm$$

6. PLANT INSTRUMENTATION AND CONTROL

In the process industry, such as this design of a plant for the production of acetic acid from methanol and CO, there is a high use of gases, hence required instrumentation control to avoid hazardous effects on the process, temperature, noise electrical equipment, fires and ignition sources and etc. all these are process hazards [14].

Pressure

Pressure pneumatic valves, control, filled as some/most pressure-relief devices, set at the maximum allowable working pressure of that potential over-pressure is relived in a controlled manner (ASME boiler and pressure vessel code, section VIII division, part UGT 125) [15].

Some marrival valves (Mechanical pressure control valve) are installed directly and indirectly on pipes/vessels carrying fluids are controlled manually [16].

Temperature

Temperature control signals are installed into reactors and heaters and even vessels such as boilers, coolers etc to help check excessive temperature that could cause open fires and other accident in the plant [15, 17]

Cost Estimation and Economic Evaluation

Cost Estimation [9]

(a) Cost of Reactor:

Annual Cost, $C = 200,000 \left[\frac{V}{100}\right]^{0.6}$ [6] $V = Volume \ of \ reactor = 372.74$ $C = \$ \frac{200,000}{300 x \, 24 \, x \, 3600} x365 \left(\frac{372.74}{100}\right)^{0.6} = \440426.66 (b) Cost of Packed Column [9]

Total cost = vessel cost + cost of packing's

olume of column =
$$\frac{\pi D^2}{4} x Z_T = \frac{\pi x \ 3.2^2}{4} x 17.2 m^3 = 138.33 m^3$$

Suppose cost per saddle intalox rings = $180/m^3$

Cost of Packing = \$180 x 138.33 = \$24900

volume cost = Bare vessel cost x MF x PF = $$100 \times 1000 \times 2 \times 1 = $200,000$ ∴ *Total cost* = \$224,900.0 2001 11

$$H_T = L_t x trays + 20\% (L_t x trays)$$

$$= (0.45 x 12) + 0.2 (0.45 x 12) = 6.48m$$

 $D_c = 3.24m$
Cost of DC = Vessel cost + cost of plates

Vessel cost = BVC X MF X PFCost of plates = No. of plate x cost per plate

$$12 x 1050 x 1.7 = $21420$$

Economic Evaluation [9]

$$Pay - Back Time = \frac{Total Investment}{Average annual Cash flow}$$

$$Production rate = \frac{350kt}{y} = \frac{350 \times 880}{400} = 770000000 lb/y = 770MMlb/yr$$

$$ISBL Capital ost = 3.450 (770)^{0.6} = 186.09M$$

$$Total investment cost = 40\% (186.09) + 186.09 = $260.52437M$$
Let the annual cash flow be \$30.38M
Thus Pay-Back-Time = $\frac{260.52437}{30.38} = 8.6yrs$

(b) Time value of money

$$i = 5\%$$

 $P = $260.52347M$

Future worth = $P(1 + i)^n$

= \$260.52437(1.05)^{8.6} = \$396.35M

(c) Annualize cost methods

$$A = \frac{P[i(1+i)^n]}{[(1+0)^n - 1]} = \frac{260.52(0.05(1.05)^{8.6}}{[(1+i)^{8.6} - 1]}$$
$$= \frac{19.82}{0.5213} = \$38.02M$$
$$ACCR = \frac{A}{P} = \frac{38.02}{260.52} = 0.1459$$

ACC = ACCR X Total Investment = 0.1459 x 400 = \$58.36M

(d) Total Annualized cost = operating cost + ACC [9, 6, 15]

= \$500+58.36 = \$558.36M

Plant Layout, Safety and Environmental Considerations [9]

Sources and Potential Exposure

- Sources of ethyleneoxide emissions to the air include uncontrolled emissions or venting with other gases in industrial settings [18]
- Other sources of ethylene oxide air emissions include automobile exhaust and its release from commodity- as well as its use as a sterilizer of medical equipment.
- The general population may be exposed to ethyleneoxide through breathing contaminated air or from smoking tobacco or being near someone who is smoking. Certain occupational groups (e.g. Workers in ethylene oxide manufacturing or processing plants, sterilization technicians, and workers involved in fumigation) may be exposed in the workplace [19].

Assessing Personal Exposure

• Tests are available to determine personal exposure to ethyleneoxide, such as the determination of ethylene oxide in the blood or the amount breathed out of the lungs [20].

Health Hazard Formation

Acute Effects

- Acute inhalation exposure of workers to high levels of ethyleneoxide has resulted in nausea, vomiting, neurological disorders, bronchitis pulmonary edema, and emphysema [21].
- Dermalorocular contact with solutions of ethyleneoxide has caused irritation of the skin and eyes in humans.
- Tests involving acute exposure of animals have shown ethyleneoxide to have high acute toxicity from inhalation exposures.

Chronic Effects (Noncancer)

- Major effects observed in workers exposed to ethyleneoxide at low levels for several years are irritation of the eyes, skin, and respiratory passages and effects to the nervous system (e.g., headache, nausea, memory loss, numbness) [22, 35].
- EPA has not established a Reference Dose (RfD) or a Reference Concentration (RfC) for ethyleneoxide [23, 34]
- The California Environmental Protection Agency (CalEPA) has established a chronic inhalation reference exposure
- Level of 0.03 milligrams per cubic meter (mg/m³) (18 parts per billion [ppb]) for ethyleneoxide based on nervous system effects in mice. The Cal EPA reference exposure level is a concentration at or below which adverse health effects are not likely to occur. It is not a direct estimator of risk, but rather a reference point to gauge the potential effects. At life time exposures increasingly greater than the reference exposure level, the potential for adverse health effects increases [24].
- ATSDR has established an intermediate inhalation minimal risk level (MRL) of 0.2 mg/m³ (0.09 parts per million [ppm]) based on an exposure below that associated with renal effects in mice. The MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. The exposure period for an intermediate MRL is from two weeks to a year [25, 37].

Reproductive/Developmental Effects

- Some evidence exists indicating that inhalation exposure to ethyleneoxide can cause an increased rate of miscarriages in female workers [26,36]
- Various reproductive effects have been noted in inhalation exposure studies of animals, including decreased

number of implantation sites, decreased testicular weights and sperm concentration, and testicular degeneration.

Cancer Risk [27, 30]

- Human occupational studies have shown elevated cases of lymphoid cancer and, also breast cancer in female workers.
- Ethyleneoxide has been shown to cause lymphoid cancer and tumors of the brain, lung, connective tissue, uterus, and mammary gland in animals exposed to ethyleneoxide by inhalation.
- EPA has concluded that ethyleneoxide is carcinogenic to humans by the inhalation route of exposure [28, 29].
- EPA additionally concludes that the weigh to evidence supports a mutagenic mode of action for ethyleneoxide toxicity [30, 31].
- EPA uses mathematical models, based on human and animal studies, to estimate the probability of a person developing cancer from breathing air containing a specified concentration of a chemical. EPA has calculated an inhalation unit cancer risk estimate of 3×10^{-3} perµg/m³ (6×10^{-3} perµpb) for ethyleneoxide for both cancer types combined (lymphoid cancer, in females, breast cancer). Taking into account the mode of action conclusion, EPA estimates that if an individual were to continuously breathe air containing ethyleneoxide at an average of 2×10^{-4} µg/m³ (1×10^{-4} ppb) over his or her entire lifetime, that person theoretically would have no more than a one-in-a-million increased chance of developing cancer as a direct result of breathing air containing this chemical. Similarly, EPA estimates that a lifetime of continuously breathing air containing 2×10^{-3} µg/m³(1×10^{-3} ppb) ethyleneoxide would result in not greater than one-in-a-hundred thousand increased chance of developing cancer. For a detailed discussion of confidence in the potency estimates, see EPA's Evaluation of the Inhalation Carcinogenicity of Ethyleneoxide [32, 33, 37].

CONCLUSION

The design of 350kt/y of Ethylene Oxide from Ethylene and Oxygen plant was carried out. The reaction chemistry considered was Ethylene and oxide at conversion rate of 0.90. Material and energy balances were carried out for the reactor, distillation column and packed column. Also, sizing of these selected units of the entire plant were carried out and importantly mechanical and Cost-estimation and economic evaluation analysis were also done and results gotten HYSYS simulation process of the plant was done and compared.

REFERENCES

- [1]. Ethylene Oxide, *Kirk-Othmer Encyclopaedia of Chemical Technology*. Elastomers, synthetic to Export Systems, 4th edition, John Wiley & Sons, Ney York, 1994, pp. 450-466.
- [2]. PP McClellan, Manufacture and Uses of Ethylene Oxide and Ethylene Glycol, *Ind. Eng. Chem.* 1950, 42(12), 2402-2407.
- [3]. S Betton and C Ruehl, Ethylene oxide purification, Journal of Chemistry and Science, 2002, 11(2), 1245-1248.
- [4]. GL Cunningham, WI Levan and WD Gwinn, the Rotational Spectrum of Ethylene Oxide, *Phys. Rev.*, 1948, 74(10), 1537
- [5]. PV Zimakov, and OH Dyment, Chapter III: Review of Individual Reactions of Ethylene Oxide, *Ethylene Oxide*, M. Khimiya, 1967, pp. 90-120
- [6]. P Dagaut, D Voisin, M Cathonnet, M Mcguinness and JM Simmie, Oxidation of Ethylene Oxide in a Jet Stirred Reactor and its Ignition in Shock Waves, *Combustion and Flame*, 1996, 156, 62-68.
- [7]. CR Ashafi, *Industrial safety and Health Management*, 5th edition prentice Hall: McGraw Hill, New York, 2003.
- [8]. H Person, A simulation model of a reactor for Ethylene oxide production. Lund University, Sweden, 2015.
- [9]. JM Coulson, JF Richardson, J Backurstand JH Harker, *Chemical* Engineering 6th edition, Butterworth Heinemann, USA, 2002.
- [10]. Han, Yuan-Zhang and Viswanathan, Hydroformylation of Ethylene Oxide, Krishnan, 20,030,032,845, 2003.
- [11]. K Weissermel and HJ Arpe, Industrial Organic Chemistry, 4th edition, Wiley-VCH, Weinheim, 2003, pp. 145-148.
- [12]. LM Neufeld and AT Blades, Kinetics of the Thermal Reactions of Ethylene Oxide, *Canadian Journal of Chemistry*, 1963, 41(12), 2956-2961.
- [13]. American Conference of Governmental, Industrial Hygienists (ACGIH).2015TLV sand BEIs. Threshold Limit, USA, 2015.
- [14]. RJ Lewis, Sax's Dangerous properties of Hazardous, Butterworth-Heinemann, USA, 2004

- [15]. K Onda, H Takeuchi and Y Okumoto, Mass transfer coefficient between gas and Liquid phases in packed columns, *Journal of Chemical Engineering Japan*, 1968 1, 56.
- [16]. R Sinnott and G Towler, Chemical Engineering Design, 5th Edition, Butter worth-Heinemann, Ney York, 2009.
- [17]. M Fingas, (2002) Handbook of Hazardous Materials Spills and Technology McGraw-Hill, London, 2002.
- [18]. DW Green and RH Perry, Perry's chemical Engineers' Handbook, 8th Edition McGraw Hill, New York, 2008
- [19]. L Octave, *Chemical Reaction Engineering*, 3rd edition, 2005, New York: John Wiley
- [20]. DD Eley, H Pines and PB Weisz, Catalytic Oxidation of Olefins, *Advances in Catalysis and Related Subjects*, Academic Press Inc., 1967, 17, pp. 156-157
- [21]. WL McCabe and EW Thiele, (1925) Graphical Design of Distillation Column Ind. Eng. Chem., 1925, 17, 605.
- [22]. MA Schuttz, DG Steward, JM Harris, SP Rosemblum, MS Shakur and DE O'brien, (2002) Reduce Costs with dividing wall columns, *Chem. Eng. Prog.*, 2002, 98 (5), 64.
- [23]. Department of Health and Human Services, Public Health Service, Centers for Disease Control and Prevention. Cincinnati, OH .http://www.cdc.gov/niosh/npg/, 2015
- [24]. JM John (2008), Hazardous Chemical, Encyclopaedia of Chemical Processing and Design, 2008, 20(2), 388-345.
- [25]. American Industrial Hygiene Association (AIHA), AIHA 2013 Emergency Response Planning Guidelines and Regulation, USA, 2013.
- [26]. Occupational Safety and Health Administration (OSHA).Occupational Safety and Health Standards, Toxic and hazardous
- [27]. In Support of Summary Information on the Integrated Risk Information System
- [28]. National Institute for Occupational Safety and Health (NIOSH). Pocket Guide to Chemical Hazards U.S.A
- [29]. Valves for Chemical Substances and Physical Agents Biological Exposure Indices Cincinnati, OH. 2015.
- [30]. Agency for Toxic Substances and Disease Registry (ATSDR). Toxicological Profile for Ethylene Oxide U.SA. Workplace Environmental Exposure Level Guides Handbook https://cfpub.epa.gov/ncea/iris/iris_documents/toxreviews/1025tr.pdf, 2013
- [31]. JS Arendt, and DK Lorenzo, Evaluating process safety in the chemical industry: A user's Guide to quantitative Analysis, Wiley-AICHE, 2000.
- [32]. CSHB, Chemical safety and hazardous investigation board preliminary findings, Americans Texas city explosion, available from www.chemsafety.gov, 2005.
- [33]. Dow, Dow's fire and Explosion Index Hazard classification Guide, *American Institute of chemical Engineers*, New York, 1994.
- [34]. RW Johnson, SW Rudy, and SD Unwin, Essential Practices for Managing Chemical Reactivity Hazards, *American Institute of chemical Engineers*, USA, 2003.
- [35]. California Environmental Protection Agency (CalEPA) (2008). Air Toxics Hot Spots Program Technical Support Document for the Derivation of Noncancer Reference Exposure Levels Appendix D3. Chronic RELs and Toxicity Summaries Using the Previous Version of the Hot Spots Risk Assessment Guidance (OEHHA 1999).
- [36]. Environmental Protection Agency. Evaluation of the Inhalation Carcinogenicity of Ethylene Oxide (CASRN), USA (IRIS). National Center for Environmental Assessment, Office of Research and Development. Washington, DC.EPA/635/R-16/350Fa.
- [37]. Public Health Service, U.S. Department of Health and HumanServices, Atlanta, GA. 1990.