Computer Aided Design of a Packed Bed Reactor for the Production of Ethylene Oxide

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Abstract The design of a plant to produce 2375mol/hr of ethylene oxide from ethylene and oxygen has been developed. Energy and material balance principles were applied to develop the functional parameters models of the reactor, columns and cooling jacket. The results generated from the simulation of the models indicates that the sizes of the columns are respectively given as: diameter of distillation and packed columns are 3.10 m and 2.50 m while the heights are 6.08 m and 16 m respectively. The volume of the reactor at required to achieve 0.9 conversion is 42.99m^3, and the diameter and length obtained for the reactor is 2.136m and 12 m. The thickness of the packed column and distillation columnare5.84 mm and 13.15 mm respectively. The heat transfer area and flow rate of the coolant of the cooling jacket are 6.97 m^2 and 51.6 kg/s respectively. The results satisfied the research topic.

Keywords Computer aided design, packed bed reactor, production, ethylene Oxide, sizing

Introduction

Ethylene oxide is an important organic chemical compound in the petrochemical industry with the molecular formula is C_2H_4O. Ethylene oxide, which has also been named oxirane by IUPAC (International Union of Pure and Applied Chemistry), is cyclic ether and the simplest epoxide: a three-membered ring composed of one oxygen atom and two carbon atoms [1-4].

Ethylene oxide is a colorless, flammable gas with a characteristic faint sweet odor. EO is primarily used for the production of ethylene glycol which is in turn used directly as an antifreeze agent in automobile vehicles. Ethylene oxide, in very small concentrations, serves as a preservative, and also as a sterilizer in medical operations [5-6]. Ethylene oxide (or propylene oxide alternatively) also finds relevance in military and warfare applications as an F.A.E (Fuel-Air Explosive) in thermobaric explosives. They are so named thermobaric explosives because their explosive force is gotten by combustion of fuel with the surrounding air [7]. This process depletes the oxygen in the surrounding air, thereby creating a vacuum and subsequent pressure difference in the surrounding. The U.S and Russia especially possess these weapons. Specific examples are the FOAB (Father of All Bombs) and MOAB (Mother of All Bombs) designed and owned by the Russian military and American military respectively [8-9].

The organic chemical compound ethylene oxide (EO) is synthesized by the oxidation of ethylene in the presence of catalysts such as platinum or silver. Ethylene glycols constitute by far the single largest group of organic compound synthesized from ethylene oxide, accounting for about 65% of the EO market in 2018 [8].

As at 2018, ethylene oxide was produced majorly in Northeast Asia, the Middle East, and North America accounting for a combined 77% of global production. A significant portion of the producers in these three regions are also integrated into the production of mono-ethylene glycol (MEG) so the consumption trend of ethylene oxide bears semblance to the global MEG production trends [10].

The production of ethylene oxide is a key process in the petrochemical industry because of the high importance of the compound as the major raw material for the production of other petrochemicals. In order to avoid: Waste of raw materials, hazards to environment, hazard to personnel, low yield of EO and excessive cost of materials, this work focuses on providing a system carefully designed to eliminate the above risks or reduce them to a barest minimum [11-12]. To achieve this, chemical engineering principles was evoked to determine the appropriate equipment and procedure for the synthesis of EO. Design of a packed bed reactor (PBR) and other key component including an absorption tower, distillation column, and a cooling jacket will be carried out to determine the following values: Height of absorption tower and distillation tower respectively, length of the reactor, diameter of the reactor, distillation column, and absorption tower respectively, mechanical design to ascertain the required thickness of the reactor and absorption tower respectively, heat transfer area of the cooling jacket, flow rate of cooling medium in the cooling jacket [13].

The aim of this study is to provide a computer aided design of a reactor for the production of ethylene oxide by direct oxidation of ethylene with oxygen. The results from this research work have significance in the following areas: Industrial trial - After carrying out design and obtaining dimensions of the key equipment, a plant for the production of EO can be fabricated using the values obtained from design, fabrication of pilot plant and subsequent scale up, simulation & optimization trials: After completing this study, a further step can be taken to optimize the reactor for higher yield of EO [14-15].

Nigeria is Africa's largest crude oil producer, and ranks sixth largest crude oil exporter in the OPEC (Organization of Petroleum Exporting Countries) bloc, but virtually all petrochemical products used in the country are imported [16]. It is therefore pertinent that the country takes advantage of its high availability of natural resources to meet its demand for petrochemical products. The natural gas, ethane, which is an associated gas in oil wells, can be synthesized to obtain ethylene which is a starting material for EO production. The high global demand for EO as an intermediary chemical makes it necessary to carry out this study [17-18]. The worldwide production of ethylene oxide currently exceeds 20 MM tons/yr [1]. Since EO is of such great importance to the world at large, it is pertinent that research such as this one is carried out. The outcome of this research will serve as a reference point for the actual fabrication of a reactor and by extension, a plant for the manufacture of EO [19-20].

This research work focuses on the computer aided design of a reactor for the production of 2375mol/hr of EO from ethylene and air in the presence of silver catalyst. The major equipment that were designed for this process include: packed bed reactor (PBR) for the conversion reaction, packed column for stripping of gases from the effluent from the PBR, distillation column for purifying and separating the EO from other components, and cooling jacket for maintaining isothermal operation of the reactor. Furthermore, mechanical design of the packed column and the reactor was carried out. A cost analysis of the equipment was also included in this work [21-22].

Materials and Methods
Materials
The materials adopted for this research work include;
- Aspen HYSYS, Ethylene Oxide Process flow diagram
- Literature data
- Industrial/plant data
- Material balance around the key components
- Energy balance
- Computation software program MATLAB Program, Microsoft Excel and PowerPoint.

Methods
The methods utilize in this research work is the design models development of the kinetics of the reactions, the distillation column, packed column and reactor model.
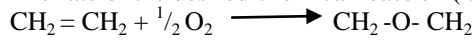
Kinetic Model Development

Assumptions

The reaction is assumed to be a first-order reaction or a pseudo first order reaction, $A \rightarrow products$. This is because the limiting reagent, oxygen, is much more deficient than the other reactant, ethylene.

The rate of the desired chemical reaction (i.e. ethylene oxide formation) is given by:

$$CH_2 = CH_2 + {}^1/_2 O_2 \longrightarrow CH_2 \text{-O-} CH_2$$

$$(r_E) = kC_\varepsilon$$

In terms of fractional conversion;   (1)

$$(r_E) = kC_{E0}(1 - X_E) \tag{2}$$

The rate constant k, is a function of temperature given by Arrhenius equation as shown in (3)

$$k = Ae^{-Ea/RT} \tag{3}$$

Substituting equation (3) into equation (2) gives;

$$(r_E) = Ae^{-Ea/RT}C_{E0}(1 - X_E)$$

Where: A is Arrhenius constant, s^{-1} $\frac{-Ea}{R}$ = ratio of the activation energy and gas constant   , $t = $ Temperature in kelvin scale

X_A Liquid phase mole fraction'

C_ε Molar concentration of ethylene oxide produced, mol/L

Reactor Design Model Development

The design models development will apply material balance principles considering the modifications/assumptions for derivation.

The performance equations are developed for Plug flow Reactor (Tubular Reactor) with the general material balance stated below:

$$\begin{pmatrix} Rate\ of\ accumulation \\ of\ materials\ within \\ the\ reactor \end{pmatrix} =$$

$$\begin{pmatrix} Rate\ of\ inflow\ of \\ materials\ into \\ the\ reactor \end{pmatrix} - \begin{pmatrix} Rate\ of\ outflow\ of \\ materials\ from \\ the\ reactor \end{pmatrix} - \begin{pmatrix} Rate\ of\ depletion\ of \\ materials\ due\ to \\ chemical\ reaction \\ within\ the\ reactor \end{pmatrix} \tag{4}$$
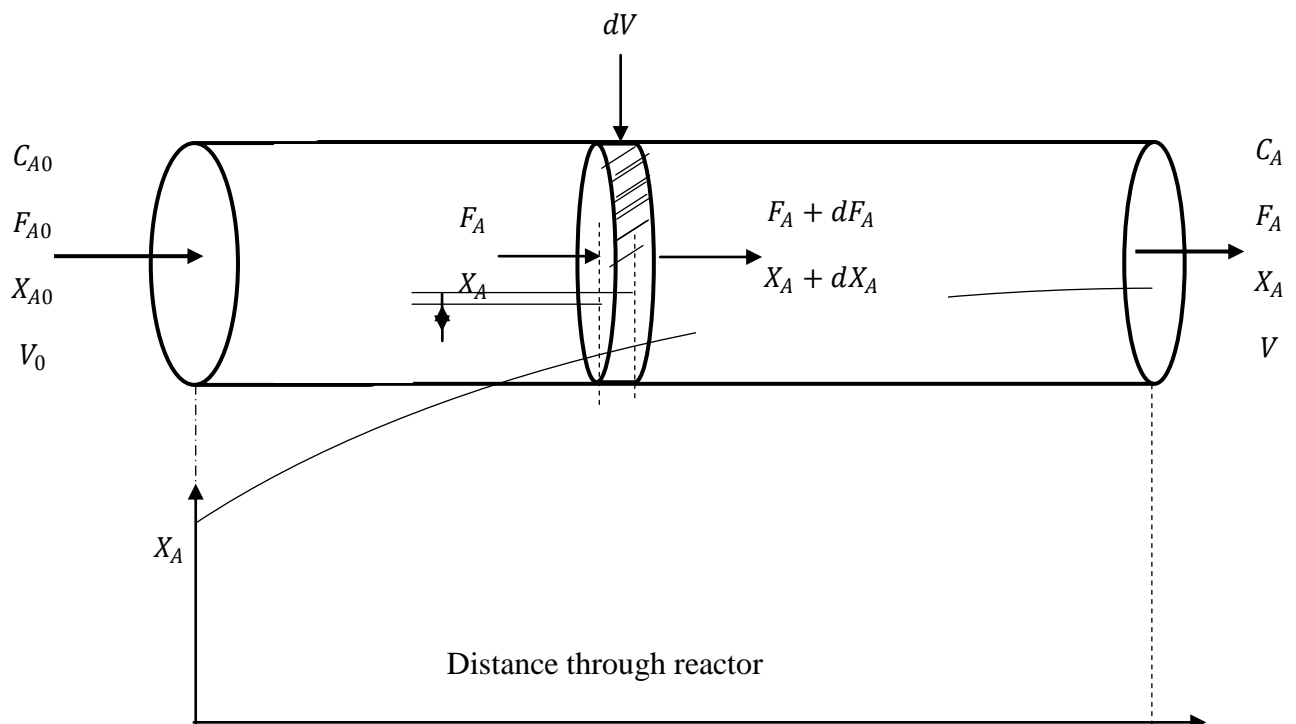

Figure 1: Schematic diagram showing the differential element of PFR

From equation (3.2), Analyzing mathematically for PFR:

$$\begin{bmatrix} Rate\ of\ inflow \\ of\ materials, \\ into\ the\ PFR \end{bmatrix} = F_A \tag{5}$$

$$\begin{bmatrix} Rate\ of\ outflow\ of \\ materials\ of\ species, A, \\ from\ the\ PFR \end{bmatrix} = F_A + dF_A \tag{6}$$

$$\begin{bmatrix} Rate\ of\ depletion\ of \\ species, A, within\ the \\ PFR\ due\ to\ chemical\ reaction \end{bmatrix} = (-r_A)dV_p \tag{7}$$

$$\begin{bmatrix} Rate\ of\ Accumulation \\ of\ species, A, within\ the\ PFR \end{bmatrix} = \frac{dN_A}{d\tau} \tag{8}$$

Substituting equations (5) to (8) into equations (4) yields:

$$F_A - (F_A + dF_A) - (-r_A)dV_p = \frac{dN_A}{d\tau} \tag{9}$$

But since *specie A* is ethylene, it shall be designated as *E* from henceforth. Eqn (9) becomes:

$$F_E - (F_E + dF_E) + (-r_E)dV_p = \frac{dN_E}{d\tau}$$

$$F_E - F_E - dF_E + (-r_E)dV_p = \frac{dN_E}{d\tau}$$

$$-dF_E + (-r_E)dV_p = \frac{dN_E}{d\tau} \tag{10}$$

Expressing F_E in terms of fractional conversion, X_A i.e. X_E for the chemical specie ethylene and substituting into equation (10)

$$F_E = F_{Eo}(1 - X_E)$$

In differential form, using Product Rule:

$$dF_E = -F_{E0}dX_E$$

Thus equation (10) becomes

$$F_{E0}dX_E + (-r_E)dV_P = \frac{dN_E}{d\tau} \tag{10b}$$

In a PFR, rate of accumulation = 0, so equation (10b) becomes;

$$F_{E0}dX_E + (-r_E)dV_P = \frac{\overset{0}{\cancel{dN_E}}}{d\tau}$$

$$(-r_E)dV_P = -F_{E0}dX_E \tag{11}$$

The functional design models are obtained from equation (11) as shown below:

a. Volume of PFR

$$dV_P = \frac{-F_{E0}dX_E}{(-r_E)} \tag{12}$$

Integrating with boundary conditions; $X_E = o$; $V_P = o$

$X_E = X_{E,F}$; $V_p = V_{PFR}$ where $(-r_E) = Ae^{-Ea/RT}C_{E0}(1 - X_E)$

$$\int_o^{V_{PFR}} dV_p = -\int_o^{X_E} \frac{F_{Eo}dX_E}{(Ae^{-Ea/RT}C_{E0}(1-X_E))}$$

$$V_{PFR} = -\frac{F_{E0}}{Ae^{-Ea/RT}C_{E0}} \int_0^{X_E} \frac{dX_E}{(1-X_E)} \tag{13}$$

$$\boldsymbol{V_{PFR} = \frac{F_{EO}}{Ae^{-Ea/RT}C_{E0}} ln\left[\frac{1}{1-X_E}\right]} \tag{14}$$

b. Space Time of PFR (τ_p)

This is mathematically stated as:

$$\tau_{PFR} = \frac{V_{PFR}}{v_o} = \frac{F_{EO}}{v_0 Ae^{-Ea/RT}C_{E0}} ln\left[\frac{1}{1-X_E}\right] \tag{15}$$

But $F_{Eo} = C_{EO}v_0$

$$\tau_{PFR} = \frac{V_{PFR}}{v_o} = \frac{1}{Ae^{-Ea/RT}} ln\left[\frac{1}{1-X_E}\right] \tag{16}$$

c. Space Velocity of $PFR(S_v)$

The space velocity of the PFR is expressed mathematically as:

$$S_{VP} = {V_o}/{V_{PFR}} = \frac{1}{\tau_{PFR}}$$

Therefore, $S_{VP} = \frac{1}{Ae^{-Ea/RT}} ln[1 - X_E]$ \hfill (17)

d. Length of the PFR

The length of the PFR is given by:

$$L_{PFR} = \frac{V_{PFR} * 4}{\pi D^2} \tag{18}$$

Recall: Volume of a cylinder $= \frac{\pi D^2}{4} \times L$

$$\boldsymbol{L_{PFR}} = \frac{4 \times F_{EO}}{\pi D^2 \times Ae^{-Ea/RT} C_{EO}} \boldsymbol{ln}\left[\frac{1}{1-X_E}\right] \tag{19}$$

e. Heat Generated Per Unit Volume of PFR

The heat generated per unit volume is given by:

$$q_p = \frac{Q}{V_p} = \frac{(-\Delta H_r)F_{EO} X_A}{V_{PFR}} \tag{20}$$

Substituting equation (14) into equation (20) yields:

$$q_p = \frac{(-\Delta H_r)F_{E0} X_A \, Ae^{-Ea/RT} C_{EO}}{F_{E0} ln\left[\frac{1}{1-X_A}\right]}$$

$$q_p = \frac{(-\Delta H_r)X_A \, Ae^{-Ea/RT} C_{EO}}{ln\left[\frac{1}{1-X_A}\right]} \tag{21}$$

f. Pressure Drop along PFR

This is only calculated for plug flow reactor since it deals with gaseous species and is the major characteristics of the reactor.

According to Sinnott *et al* [20], has expressed the pressure drop in a tubular flow system as:

$$\Delta p = \frac{8fl\rho u^2}{2D} = \frac{4fl\rho u^2}{D} \tag{22}$$

Where $f = \frac{0.04}{Re^{0.16}}$ \hfill (23)

But $Re = \frac{\rho u D}{\mu'}$ \hfill (24)

Combining all the 3 (three) equations gives

$$\Delta P = \frac{0.16 L\rho^{0.84} u^{1.84} \mu^{0.16}}{D^{1.16}} \tag{25}$$

Where:

$\rho = density \ of \ the \ flowing \ material, [kg/m^3]$
$D = Diameter \ of \ the \ PFR, [m]$
$L = Length \ of \ the \ PFR, [m]$
$\mu' = mean \ fluid \ viscosity \ [Ns/M^2]$
$u = Mean \ superficial \ velocity, [m/s]$
$\Delta P = change \ or \ pressure \ drop \ per \ bars, [KP_a]$
$Re = Reynold's number \ [-]$

Equation (25) becomes:

$$\Delta P = \frac{0.16 L_{PFR}\, \rho^{0.84} \mu^{,0.16} u^{1.84}}{D^{1.16}} \tag{26}$$

$$\Delta P = 0.16 \left\{ \frac{\left\{ \left[\frac{4*F_{AO}}{\pi (0.4)^2 \mu} \right] \ln(1-X_A) \right\}^{1/3} \rho^{0.84} \mu^{,0.16} u^{1.84}}{D^{1.16}} \right\} \tag{27}$$

Where $\mu = k_o \exp(-\beta t^m) P_T$ as already been defined

And $D = \frac{L_{PER}}{2.5}$

Distillation Design Models
Material balance in the column

F = D + B $\tag{28}$

Species balance:

For Ethylene oxide,

$X_f F = y_f D + X^1_f B$ $\tag{29}$

For the bottom column balance

$X_W F = Y_W D + X^1_W B$ $\tag{30}$

Combining equations (29) and (30) gives various flow rates i.e. D and B since F is given.

$$D = \frac{F(X_f - X^1_f)}{y_D - X^1_f} \tag{31}$$

$$B = F - D = F - \frac{(F(X_f - X^1_f))}{Y_D - X^1_f}$$

$$B = \frac{F(Y_D - X^1_f) - FX_f + FX^1_f}{Y_D - X^1_f} \tag{32}$$

$$B = \frac{(F(Y_D - X_f)}{Y_D - X^1_f} \tag{33}$$

Vn = RD + D = D (R+1) $\tag{34}$

Ln = RD $\tag{35}$

Since the mixture enters below its boiling point, then q must be determined.

$$q = 1 + \frac{Cp_{av}(T_{fs} - T_f)}{\lambda_{av}} \tag{36}$$

Lm = Ln + q_f $\tag{37}$

Vm = Lm – B $\tag{38}$

Operating line Equations

U_{OL}: $y_n = \frac{Ln}{Vn} x_n + \frac{D}{Vn} x_f$ $\tag{39}$

LOL: $y_m = \frac{Lm}{Vm} x_m - \frac{B}{Vm} x'_f$ $\tag{40}$

Determination of Actual number of plates from theoretical ones

- The equilibrium data is plotted as y1 Vs x1 to get the McCabe Thiele diagram which will be used to get the theoretical plate number.
- Using (assuming) Efficiency of the column to be 60% or according to Lewis, 1936, the efficiency is determined using Murphree plate efficiency (E_m)

$$\varepsilon_0 = \frac{Log\,(1 + EmV\,(MVn - 1))}{Log\,(M\frac{Vn}{Ln})} \tag{41}$$

Thus,

No of actual plates $= \frac{No\ of\ Theoritical\ plates}{Efficiency}$ or

No of actual plates $= \frac{No\ of\ Theoritical\ plates}{assumed\ Efficiency\ (60\%)}$ $\tag{42}$

Design Equations for the Diameter of the column, DC.

$$F_{LV} = \frac{Ln}{Vn} \sqrt{\frac{\rho v^\varepsilon}{\rho L^\varepsilon}} \tag{43}$$

$$F_{LV} = \frac{Lm}{Vm}\sqrt{\frac{\rho v^w}{\rho L^w}}$$

From Sinnott *et al*, 2009, K_1 is obtained.

$$\frac{Correction\ of\ k1\ values\ (K')}{0.2}$$

$$k_1' = k_1(\sigma/0.02)0.2 \tag{44}$$

Flooding vapour velocity, m/s is calculated as thus;

$$U_f = k_1'\sqrt{\frac{\rho l - \rho v)}{\rho v}} \tag{45}$$

Calculation of minimum vapour velocity through the holes (based on the area), m/s, U_n

$$U_n = \frac{\{K_2 - 0.90\ (25.4 - dn)\}}{(\rho v)^{1/2}} \quad [20] \tag{45}$$

% flooding $= Un/Uf$

Suppose we have 85% flooding, then

$$Un = 85\%\ U_f \tag{46}$$

Calculation of volumetric flow rate

$$V_1 = \frac{Vn * M_i}{\rho v} \tag{47}$$

Calculation of column area, (Ac)

$$An = V^1/U_n \tag{48}$$

$$Ac = \frac{An}{0.88} \tag{49}$$

$$Dc = (\frac{4\ Ac}{\pi})\ ½ \tag{50}$$

Design calculation for the column height

Taking 20% allowance for the entire column

$Hc = $ (No of trays/ plates)$\times \hat{t}$

Where:

    $\hat{t} = $ plate spacing, 0.5m

$$H_T = \text{(overall height)} = H_C + 20\%\ H_C \tag{51}$$

Design Equation for Packed Column

The scrubber in the process flow diagram is designed as a packed column.

The packed column is used to scrub gas particles such as CO_2 produced inside the reactor.

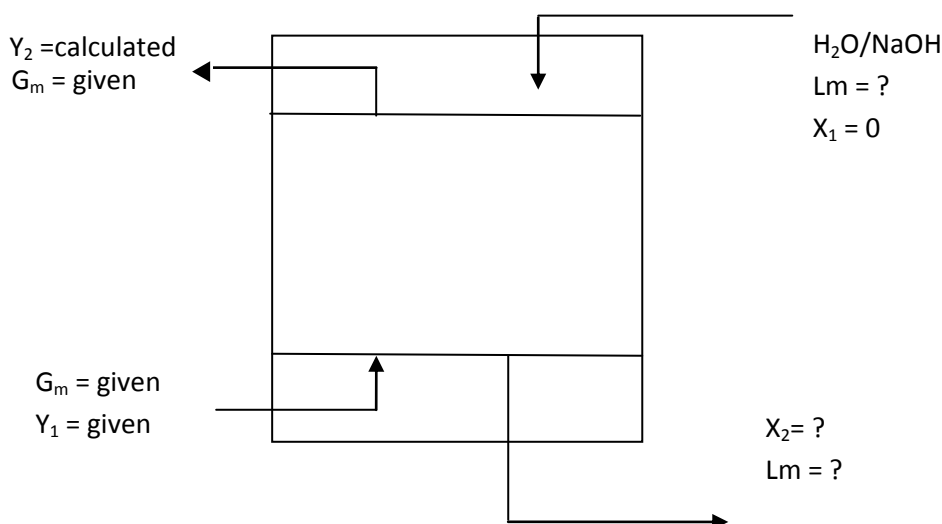Column material balance is as thus;

$Y_2 = $ calculated

$G_m = $ given

$H_2O/NaOH$

$Lm = ?$

$X_1 = 0$

$G_m = $ given

$Y_1 = $ given

$X_2 = ?$

$Lm = ?$

Figure 1: Schematic diagram for material balance in a packed column

Material balance of packed column

Flow rate in = flow rate out at steady-state, accumulation rate = 0

$GmY_1 + LmX_1 = GmY_2 + LmX_2$

But $X_1 = 0$, assumed pure solvent

$GmY_1 = GmY_2 + Lm\ X_2$

$GmY_1 - Gm\ Y_2 = Lm\ X_2$

$Gm\ (Y_1 - Y_2) = Lm\ X_2$

$X_2 = \dfrac{G_m}{L_m}(Y_1 - Y_2)$

But

$Y_1 - Y_2 = 98\%\ Y_1 = 0.98\ Y_1$

$X_2 = 0.98Y_1\dfrac{G_m}{L_m}$ (52)

Also, knowing the amount of gas remaining in the waste solvent, X_2 can be gotten in other to calculate for Lm

$M = {Y_1}/{X_2}$ (53)

$X_2 = \dfrac{\frac{W_1}{M_G}}{\frac{W_1}{M_G} + \frac{W_2}{m_s}} = \dfrac{n_1}{n_1 + n_2}$ (54)

Where

n_1 = mole fraction of gas absorbed at the bottom column at the exit.

n_2 = mole fraction of the solvent at the exit

W_1 = mass fraction of the gas at exit.

W_2 = mass fraction of the solvent at the exit

$M = \dfrac{G_m}{L_m}$ can be obtained and rated to get, N_{0G} based on the relationship between $m\dfrac{G_m}{L_m}$ and N_{OG}

$N_{OG}\dfrac{1}{1-\left[\frac{mG_m}{L_m}\right]} ln\ \left[\left\{1 - \dfrac{mG_m}{L_m}\right\}\dfrac{y_1}{y_2} + \dfrac{mG_m}{L_m}\right]$

Where N_{OG} = overall number of transfer unit

Column Diameter Design

$Gm = \dfrac{Gi}{3600_s}\ (kmol/_s)$

Where:

Gi = mass flow rate gotten from material balance.

$Lm = {Li}/{3600}\ (kmol/_s)$

Where

$Li = 0.98\ \dfrac{Y_1 G_m}{X_2}$ (55)

Select material type of packing i.e. 25mm Raschings rings ceramics

Packing factor Fp = 525 m^{-1}

$\rho^g = \dfrac{M_{mix}}{22.4}\ \text{x}\ \dfrac{T}{T_f} = \dfrac{M_{mix}}{22.4}\ \text{x}\ \dfrac{273}{(30+273)}$ (56)

ρl = density of the solvent known or gotten from data (literature)

$F_{Lv} = \dfrac{L_m}{G_m}\ \sqrt{\dfrac{\rho g}{\rho l}}$ (57)

Taking 20mm of water per packing of pressure drop

K_4 is obtained from FLV as above.

$Gi^* = \left\{\dfrac{K_4 \rho\ (\rho_L - \rho_g)}{13.1\ Fp\ (^{\mu L}/_{\rho L})^{0.1}}\right\}^{1/2}$, kg/s.m^2 (58)

Thus, ac = column area is calculated as thus;

$ac = \dfrac{G_m}{Gi^*}$, m^2 (59)

Hence, column diameter is given

$$D_C = (\frac{4ac}{\pi})\ ½,\ m \tag{60}$$

Estimation of H_{OG}, hence Height of column

Onda *et al* (1968) stated design models for the estimation of overall height of gas transfer unit which are given as:

Given: D_L (Diffusivity of liquid), m^2/s

D_v = Diffusivity of vapour, m^2/s

μv = Viscosity (vapour), Ns/m^2

$$\frac{a_w}{a} = 1 - \exp\ (-1.45\ (\sigma_c/\sigma_L)^{0.75}\ (\frac{Li^*}{\mu l})^{0.1}\ (\frac{Li^*a}{\rho^2 Lg})^{-0.05}\ (Li^{*2}/\rho_l\sigma_l\mu_l)^{0.2}) \tag{61}$$

Where;

a = 194 m^2/m (actual area of packing) per unit volume, see table 11.2 vol 6, chemical Engineering design Sinnott *et al,* 2009).

a_W= Effective interfacial area of packing per unit volume, m^2/m^3

σ_c = critical surface tension (61 x 10^{-3} N/m)

σ_L = surface tension of liquid, N/m

g = acceleration due to gravity, 9.81 m/s^2

Determination of mass transfer coefficients for both liquid and gas K_L and K_G

$$K_L = (\rho L/\mu_L g)\ 1/3 = 0.0051\ (\frac{Li^*}{a_w \mu_L})^{2/3}\ (\frac{\mu_L}{\rho_L D_L})^{1/2}\ (adp)^{-0.4} \tag{62}$$

$$K_G = (\frac{RT}{a D_v}) = K5\ (\frac{Gi^*}{a_{\mu v}})\ 0.7\ (\frac{\mu_v}{\rho_g D_v})^{1/3}\ (adp)^{-2} \tag{63}$$

Where:

K_5 = 5.23, for packing size above 15mm and for sizes below 15mm.

R = 0.08314 bar m^3/kmol.k.

$Li^* = \frac{L_m}{a_c}$, $kmol/m^2 s$

$Gi^* = Gi^*/M_S$, $kmol/m^2$.s

P = given total pressure, atmospheric (101.325 kPa).

Determination of liquid and gas height of transfer unit, H_L and H_G

$$H_L = \frac{L_m}{K_L a_w C_t},\ m \tag{64}$$

Where

$$C_t = \frac{\rho_L}{M_s} \tag{65}$$

Where Ms = molar mass of solvent.

$$H_G = \frac{G_m}{K_G a_w P} \tag{66}$$

$$H_{OG} = H_G + M\frac{G_m}{L_m} H_L \tag{67}$$

$$Z = N_{OG} H_{OG} \tag{68}$$

$$Z_T = Z + 30\% Z \tag{69}$$

Definition of terms

Z_T = Total height of the packed column

R= Ideal gas constant

M = Slope of the equilibrium line

Ct = Total concentration, $kmol/m^3$

dp = packing size, mm.
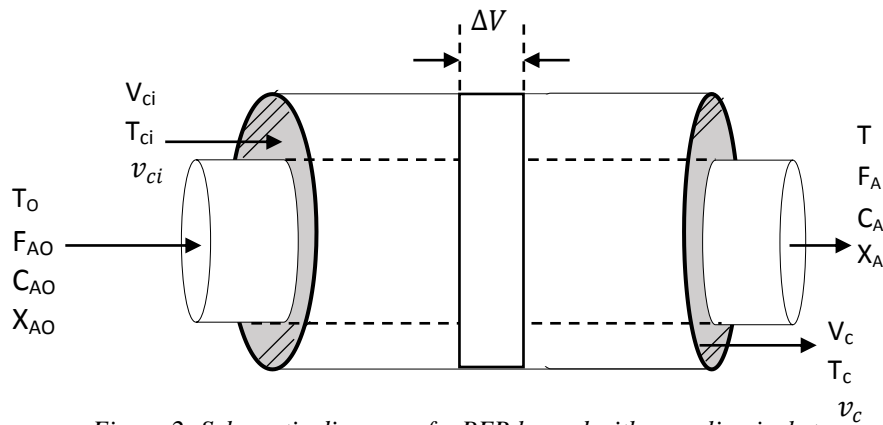
Design of a Cooling Vessel

Figure 2: Schematic diagram of a PFR lagged with a cooling jacket

Material balance around the cooling jacket

$$\left\{\begin{array}{c}\text{Rate of accumulation of materials}\\ \text{within the cooling vessel}\end{array}\right\}$$
$$= \left\{\begin{array}{c}\text{Rate of inflow of materials}\\ \text{into the cooling vessel}\end{array}\right\} - \left\{\begin{array}{c}\text{Rate of outflow of materials}\\ \text{from the cooling vessel}\end{array}\right\} \tag{70}$$

Mathematically; $\frac{dm}{dt} = \frac{m}{t}$ *entering* $- \frac{m}{t}$ *leaving* $\tag{71}$

But $\rho = \frac{m}{V}$ $\therefore m = \rho V$ $\tag{72}$

Also $v_c = \frac{m^3}{t}$ $\qquad \rho = \frac{kg}{m^3}$

$\therefore v_c \rho = \frac{m^3}{t} \times \frac{kg}{m^3} = \frac{mass}{time}$

$\therefore \frac{m}{t} = v_c \rho$ $\tag{73}$

Substituting (70) and (71) and (72) into (73) gives;

$\frac{d\rho_c V_c}{dt} = v_{ci}\rho_{ci} - v_c\rho_c$ $\tag{74}$

Assumptions:
1) Density of coolant, ρ_c is constant
2) Volume of the system is constant

$\therefore \frac{d\rho_c Vc}{dt} = v_{ci}\rho_c - v_{ci}\rho_c$ $\tag{75}$

$\Rightarrow \frac{d\rho_c Vc}{dt} = v_{ci} - v_{ci}$ $\tag{76}$

At steady state; $\frac{d\rho_c Vc}{dt} = 0$

$\therefore \boldsymbol{v_{ci} = v_{ci}}$ $\tag{77}$

Equation (84) represents the material balance for a cooling jacket.

Energy Balance on the cooling vessel
Assumptions:
Kinetic and potential energy and
Shaft work are negligible

Case 1: When the temperature of the coolant remains constant with volume

$$\begin{Bmatrix} \text{Rate of accumulation of} \\ \text{energy within the vessel} \end{Bmatrix} - \begin{Bmatrix} \text{Rate of inflow of} \\ \text{energy into vessel} \end{Bmatrix}$$

$$- \begin{Bmatrix} \text{Heat entering via heat transfer} \\ \text{from vessle walls} \end{Bmatrix} = \begin{Bmatrix} Rate\ of\ outflow\ of\ heat \\ form\ vessel \end{Bmatrix} \tag{78}$$

On basis of the enthalpies of the fluids $\frac{dH}{dt} = \frac{H}{t}$ enterting $- \frac{H}{t}$ leaving $\tag{79}$

But $H = mC_P\Delta T = \rho v C_P \Delta T$ $\tag{80}$

$v\rho_c = \frac{\text{mass}}{\text{time}}$ $\tag{81}$

Substituting (80) and (79) into (78) gives;

$$\frac{d(\rho_c V_c C_{P_c} T_c)}{dt} = v_{ci}\rho_{ci}C_{Pci}(T_{ci-}T_C) - v_c\rho_c C_{Pc}(T_{ci-}T_C) - Q \tag{82}$$

Assuming constant density, volume, and heat capacity we have;

$$\frac{(\rho_c V_c C_{P_c})dT_c}{dt} = v_c\rho_c C_{Pc}[T_{ci-}T_C] - Q \tag{83}$$

$$Q = UA(T_C - T) \tag{84}$$

Dividing all through by $V_c\rho_c C_{Pc}$ and putting in (84) gives;

$$\frac{dT_c}{d\tau} = \frac{v_c}{V_c}(T_{ci} - T_c) - \frac{UA(Tc-T)}{Vc\rho_c C_{Pc}} \tag{85}$$

Equation (85) represents the model for the energy balance of a cooling jacket when temperature of coolant changes with time.

Case II: Energy Balance for variable temperature (with volume) cooling jacket

For plug flow reactors and at low or moderate flow rates, the cooling medium used in the cooling jacket or vessel carries across the volume or length of the cooling vessel. To represent this situation with a mathematical model, a cross-sectional area of the cooling jacket is considered.

Thus energy balance is written as;

$$\begin{Bmatrix} \text{Rate if accumulation of energy} \\ \text{within vessel} \end{Bmatrix} - \begin{Bmatrix} \text{Rate of inflow of} \\ \text{energy into vessel} \end{Bmatrix} - \begin{Bmatrix} \text{Rate of outflow of} \\ \text{energy from vessel} \end{Bmatrix} =$$

$$\begin{Bmatrix} \text{Rate of heat transferred} \\ \text{to vessel walls and surrounding} \end{Bmatrix} \tag{86}$$

$$\frac{d\rho_c C_{pc} T_c v_c}{dt} = v_c\rho_c C_{pc}T_{cv} - v_c\rho_c C_{pc}T_{cv+dv} - UA(T - T_a)dV \tag{87}$$

At steady state, accumulation term = 0 arranging like terms in equation (87)

$$0 = v_c\rho_c C_{pc}T_{cv} - v_c\rho_c C_{pc}T_{cv+dv} - UA(T - Ta)dV \tag{88}$$

Taking limit as $dV \to 0$ in eqn (88) we have:

$$v\rho_c c_{pc}\frac{dT}{dV} = UA(T - T_a) \tag{89}$$

Divide all through by $v_c\rho_c c_{pc}$ gives;

$$\frac{dT}{dV} = \frac{UA(T-T_a)}{vc\rho_c C_{Pc}} \tag{90}$$

Equation (90) is the energy balance for a cooling jacket with variable temperature.

Determination of Key Operational Parameters of a Cooling Jacket

For all heat transfer processes, the general equation is expressed as;

$$Q = UA\Delta T \tag{91}$$

Where Q = rate of heat output from reactor

U = overall coefficient of heat transfer.

ΔT = temperature difference in the cooling or heating medium before and after each operation. If the medium changes temperature as it moves through the vessel or system, then a logarithmic mean temperature is used.

A = area of heat transfer

❖ The primary objective of all design of heat transfer equipment is to ascertain the area of heat transfer, as necessary to deliver the required cooling or heating to the system.

❖ Secondly, the flow rate of coolant or cooling medium must be sufficient to cause the required cooling to the jacket reactor, yet not higher than necessary as this will in core more cost of operation arising from higher energy input.

Correlations and Formulas for Agitated Cooling Vessel/Cooling Jacked

a). The Over-all Heat Transfer Coefficient.

This value is obtained by taking into account all the resistances to heat transfer in the agitated vessel system. It is expressed as the sum of the reciprocal of all resistance to heat transfer.

Overall heat transfer coefficient for agitated vessel (general case) is:

$$\frac{1}{u_D} = \frac{1}{h_C} + \frac{1}{h_{DM}} \tag{92}$$

The above terms are explained in the next session.

Where; $u_D \Rightarrow$ overall heat transfer coefficient

$\qquad h_C \Rightarrow$ heat transfer coefficient of jacket

$\qquad h_{DM} \Rightarrow$ heat transfer coefficient for cooling deposits

ai). Jacket Side Heat Coefficient

For liquid coolants (e.g. water, organic solvents), Heat transfer coefficient of the jacket side is expressed as;

$$(N_{NU}) = A_1 (N_{RE})0.8x\ (N_{PR})6XN(\rho/\rho_{cw})0.14 \tag{93}$$

Where N_{NU} = Nusselt number of coolant $\Rightarrow h_c D_c\ /K_c$ $\qquad$ (94)

N_{RE} = Reynold's number for coolant $\Rightarrow D_c\ x\ v\ x\ \rho_c$ $\qquad$ (95)

N_{RE} = Prandlt number of coolant $\Rightarrow C_{cp}\ x\ \cup_c\ /\ K_c$ $\qquad$ (96)

Also Note; h_c = heat transfer coefficient of coolant fluid, W/m^{2}k^{-1}

$\qquad D_c$ = Cross flow diameter of the coolant fluid.

$\qquad v$ $\ $ = Fluid velocity m/s

$\qquad \cup_c$ $\ $ = Viscosity of cooling fluid or coolant, N/s/m^2

$\qquad N_{cw}$ = Viscosity of coolant at jacket wall temperature

$\qquad C_{cP}$ Coolant fluid heat capacity at the average jacket temperature, J/K/Kg or J^{-1} K^{-1} Kg

$\qquad \rho_c$ $\ $ = Coolant density at average jacket temperature, Kg/m^3

$\qquad b$ $\ $ = Recommended constants for equation (3.23) for cooling processes b=0.3

$\qquad$ A1 = 0.0265 for cooling

$\qquad$ Rearranging the above relations given;

$$\boldsymbol{h_C = (K_{C\times}A_1/D_C)\times(D_CV\rho_C/\mu_C)exp\frac{2}{3}\times(C_C\times U_C/K_C)expb\times\left(\frac{\mu_C}{\mu_{CW}}\right)} \tag{97}$$

$\boldsymbol{h_{DM}}$ **is gotten from tables as shown below;**

Table 1: Typical values for typical fouling, $R_D = \frac{1}{h_{DC}}$, m^{2}K/W

Source of water	Liquid velocity < 0.glm/s	Liquid velocity > 0.9lm/2
Sea water	0.0005	0.0005
well water	0.001	0.001
river water (Clean)	0.002	0.001
River water (moddy)	0.008	0.006
Rain	0.001	0.001

NB: In cases where the operating pressure is not high and the vessel wall is made of materials such as steel, copper etc., the vessel wall thickness will be relatively small and thermal conductivity relatively high. Thus, the ratio of thickness to thermal conductivity will be a magnitude smaller than other resistances and is thus assumed negligible.

Typical values for overall heat transfer coefficient for jacketed system is shown below.

Table 2: Typical overall coefficients for jacketed vessels or reactors

Duty	U $(Wm^2\,C^{-1})$	Materials
Heating	400	Carbon and Stainless Steel
Cooling	350	Carbon and Stainless Steel
Chilled Service	150	Carbon and Stainless Steel
Cooling (on agitation)	70	Carbon and Stainless Steel

Let U be taken as $200\ Wm^2\,C^{-1}$

b). Rate of Heat Output from the Reactor, Q

The heat generated by the reaction in the plug flow reactor is the amount of heat that must be removed by the cooling jacket to keep the process isothermal.
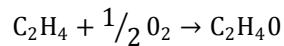
The heat of reaction, Q is calculated with the

$\pm\,\Delta\,H_R = \sum(\Delta\,H_f\ \text{products}) - \sum(\Delta H\ \text{reactants})$

$\Delta H_f \Rightarrow$ heat of formation

$\Delta H_{R\,\Rightarrow}$ heat of reaction

The balanced chemical equation for ethylene and oxygen reaction is;

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

From tables (Perry & Green, 2007)

ΔH_f of ethylene oxide $= -52.6KJ/mol$

ΔH_f of thylene $= 52.47KJ/mol$

ΔH_f of oxygen $= KJ/mol$ (pure element)

$-\Delta\,H_R = 1(-52.6) - \left[{}^1/_2\,(0) + 1\,(52.47)\right]$

$-\Delta\,H_R = 105.7KJ/mol$

$-\Delta H_R$ designates that this is an exothermic reaction.

Also from equations 22 and 23 we have that;

$q_p = \dfrac{Q}{V_p} = \dfrac{(-\Delta H_r)F_{EO}\,X_A}{V_{PFR}}$

$q_p = \dfrac{(-\Delta H_r)F_{E0}X_A\ Ae^{-Ea/RT}C_{EO}}{F_{E0}\,ln\left[\frac{1}{1-X_A}\right]}$

$q_p = \dfrac{(-\Delta H_r)X_A\ Ae^{-Ea/RT}C_{EO}}{ln\left[\frac{1}{1-X_A}\right]}$

Therefore, the value of Q is calculated as

$Q = q_p\ x\ v_R$ (98)

(c). Logarithmic Mean Temperature, ΔT

For most industrial process, ΔT for efficient heat transfer processes in cooling jackets is taken t is as around 10 ºC-50 ºC. The correlation of logarithmic mean temperature difference is given as;

$LMTD = \dfrac{\Delta T_1 - \Delta T_2}{In\left(\frac{\Delta T_1}{\Delta T_2}\right)} = \dfrac{\Delta T_1 - \Delta T_2}{In\,\Delta T_1 - In\,\Delta T_2}$

Where $\Delta T_1 =$ hot fluid temperature $(inlet - outlet)$

$\quad\quad\ \Delta T_2 =$ cold fluid temperature $(inlet - outlet)$

d). Required Flow Rate of Coolant

Flow rate of coolant in heat transfer is calculated thus:

$Q = \dot{m}c_p\,\Delta T$ (99)

Therefore, $\dot{m} = \dfrac{Q}{C_P\Delta T}$ (100)

Where $\dot{m} =$ mass flow rate of coolant

d) Heat Transfer Area, A

The heat transfer area of the cooling jacket is calculated with the equation,

$$A = \frac{Q}{v \Delta \tau} \tag{101}$$

e) Flow Width of Cooling Jacket, W

The spacing between the cooling jacket and the reactor wall is called the flow width. Its value depends of the size of the vessel.

Table 3: Typical Values for Flow Width in Jacketed Vessels

Vessel Type	Flow Width (mm)
Small Vessels	50m
Average Size Vessels	150-170
Large Vessels	3000

f) Volume of Jacket, V_{jc}

$$V_{jc} = w \times A \tag{102}$$

where w is the flow width of the cooling jacket.

Typically, the value of w is taken as 0.3 m for large reactors.

Input Parameters

Table 4: Input Parameters [23]

Parameter	Value
Feed molar flowrate (ethylene), F_{E0}	733.2003 mol/s
Feed inlet (oxygen), F_{O0}	100 mol/s
Rate constant, k	3.0929 mol/m^{3}s
Feed concentration (ethylene) C_{E0}	12.9942 mol/m^3
Inlet temperature of ethylene	230 °C
Inlet temperature of oxygen	270 °C
Inlet pressure of ethylene	210 pisg
Inlet pressure of oxygen	230 psig

Results

Table 5 demonstrates the results generations in MS Excel for the functional parameters of the tubular reactor with the fractional conversion to determine the performances of the reactor to produce formaldehyde from methanol. The rate values are in terms of kmol/s.m^3; the volume of the reactor is measured in cubic meter; the space time (s); the space velocity (per sec) and length and diameter of the reactor in meter.

Table 5: Results of the Simulated Plug Flow Reactor

X_E	V_{PFR} (m^3)	L_{PFR} (m)	S_T (s)	S_V ($1/S$)	q_{PFR} (KJ/s)
0.1	1.9676	0.5866	0.03407	29.3513	1648.79
0.2	4.1671	1.2424	0.07214	13.8619	2096.83
0.3	6.6608	1.9859	0.1153	8.6730	2454.13
0.4	9.5395	2.8441	0.1652	6.0533	2454.13
0.5	12.9442	3.8592	0.2241	4.4623	2762.39
0.6	17.1114	5.1016	0.2963	3.3750	333.80
0.7	22.4837	6.7034	0.3893	2.3687	3514.38
0.8	30.0556	8.9609	0.52037	1.9217	3782.29
0.9	42.9999	12.8201	0.74447	1.3432	4016.43

Tables 5 shows the results generations in MS Excel for the functional parameters of the tubular reactor with the fractional conversion to determine the performances of the reactor to produce ethylene oxide from oxygen and ethylene. The volume of the reactor is measured in cubic meter; the length of the reactor the space time (s); the space velocity (per sec), and the heat generated per unit volume of the reactor.

Table 6: Design and Thickness of the PFR and the Columns

Parameter	PFR	Distillation Column	Packed Column
Diameter	2.136m	3.10m	2.5m
Height	12m	6.08m	16m
Thickness	−	13.15mm	5.84mm
Volume	42.99m^3	45.90m^3	78.55m^3

Table 6 shows the results obtained from the manual calculations for the sizes of the key equipment namely the reactor and the columns.
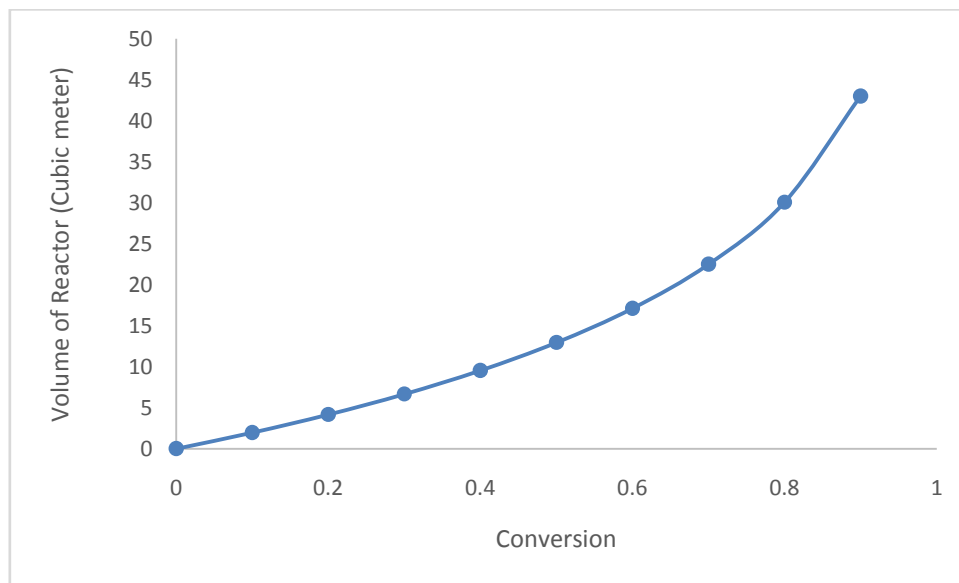
Profile Plots

Figure 3: Variation of Volume of Plug Flow Reactor with fractional conversion

Figure 3 depicts the variation of volume of plug flow reactor for ethylene oxide production from ethylene and conversion. The volume increases exponentially from 0m^3 to 42.9 m^3 as conversion too increases from 0-0.9. The increase in volume is achieved as a result of decrease in the rate values. Production of ethylene oxide is favourbale at higher conversion and lower rates.
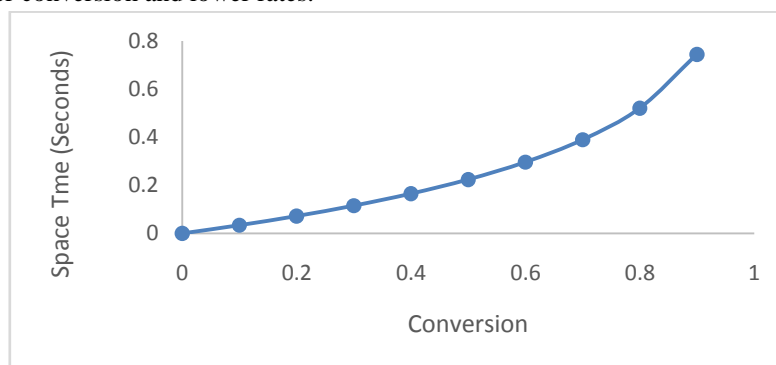

Figure 4: Profile of Space Time of the Reactor versus Conversion

Figure 4 depicts the variation of space time of tubular reactor varying with conversion. The profile of the space time is exponentially increased with conversion starting from 05-0.035sec when X_A=0-0.9 respectively. Space time is defined as the time taken for one reactor feed volume converted to product. From the results, the space

time values are very small meaning the reaction is a fast one. Increasing the space time values, leads to increase in the value of the reactor and higher yields of the product formed.
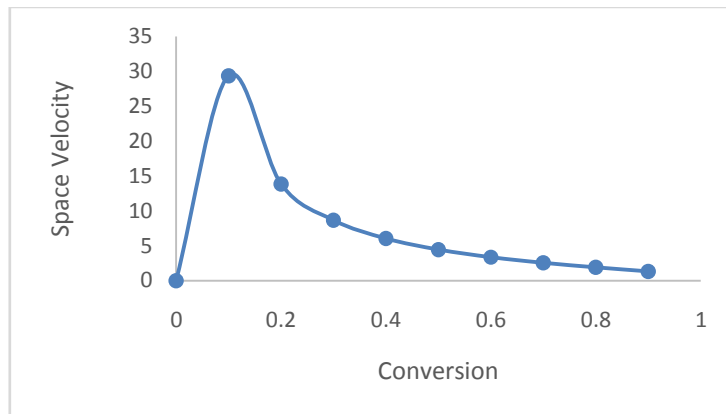

Figure 5: Graph of Space Velocity versus Conversion

Figure 5 shows the graph of space velocity varying with conversion. The inverse of space time gives the space velocity's values. The space velocity's values are higher and increases from 0-30s^{-1} when conversion increases too from 0-0.1 and then drops exponentially from 30-15s^{-1} when conversion increases from 0.1-0.9. The space velocity should be reduced to achieve higher yield at lower cost as shown from the profile plot.
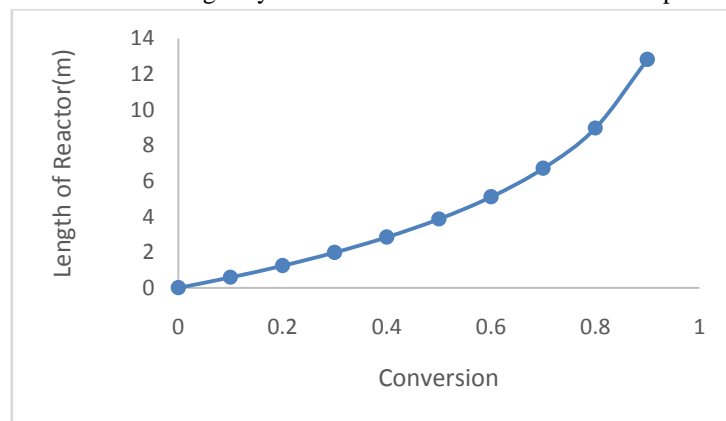

Figure 6: Profile of length of plug flow reactor versus conversion

Figure 6 demonstrates the profile variation of length of the reactor varying with conversion. The results in the profile gives an increase of the length of reactors value with conversion increase. The length of reactor values increased from 0m -12m due to increase in conversion from 0-0.9. The increase in length resulted to increase in volume of the reactor and decrease in the rate of reaction values. The volume of the reactor is a function of length and rate of reaction.
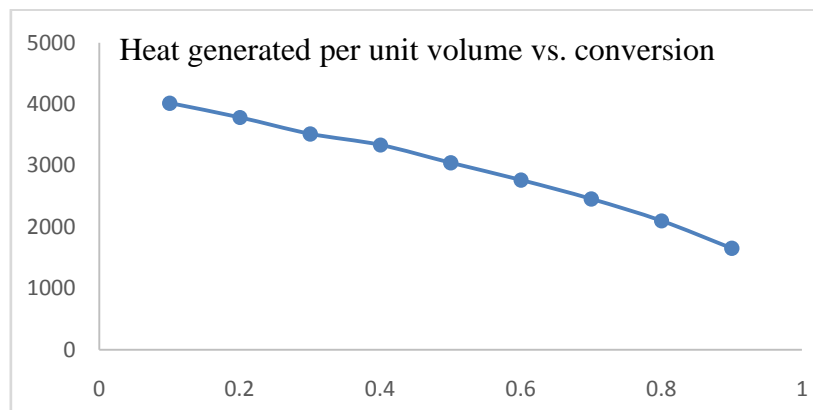

Figure 7: Profile of heat generated per unit volume of reactor versus conversion

Figure 7 shows the profile plot of heat generated per unit volume against fractional conversion. It can be observed that the heat output diminishes as the reaction goes to completion. Heat output is 4016 KJ/s at conversion of 0.1 and drops to 1671 KJ/s at 0.9 conversion.
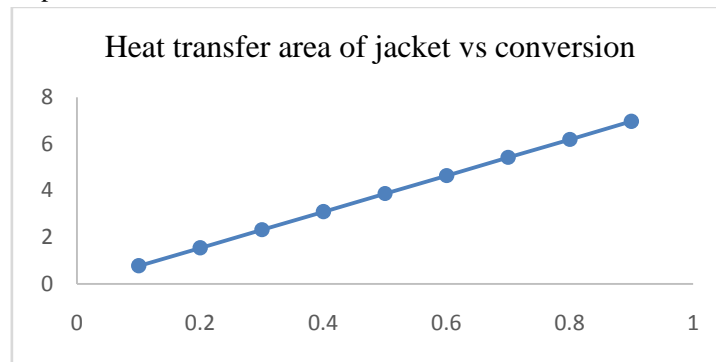

Figure 8: Profile of heat transfer area against conversion

Figure 8 shows that the area of heat transfer needed to cool the reactor increases as conversion increases. The higher the conversion of reactants, the more heat is generated and thus more area of heat transfer of the cooling jacket needed to keep the process isothermal. The area increases from $0m^2$ to $6.9m^2$ as conversion increases from 0 to 0.9.
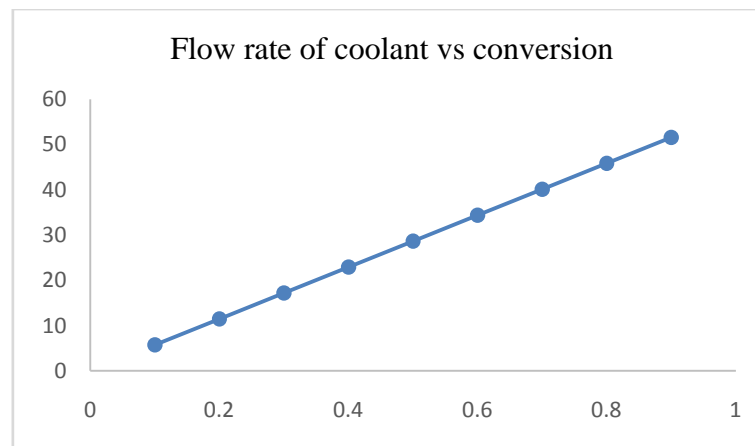

Figure 9: Profile of flow rate of coolant against conversion

Figure 9 shows that the flow rate of coolant needed to absorb the heat generated by the reactor is a function of how much reactants are converted. The flow rate increases from 0 to 51.6 kg/s as the conversion increases from 0 to 0.9.

Conclusion

The research work for the design of 2375mol/hr plant of ethylene oxide production from ethylene has been carried out. The plant takes into account the design of four main equipment i.e. cooling jacket, the reactor, the distillation column, and packed scrubber) columns in the ethylene oxide plant manually. The design equations for the columns were developed for the sizing of the columns to be determined. The performance model and functional parameters models of the reactor was developed for performance evaluation process. The design models developed were simulated manually and also using software program (MS EXCEL) using literature data. Performance table was generated and the sizing of the reactor and columns were also product as shown in table 4.1. Profiles for the functional parameters of the reactor were obtained from the simulated results as shown in the research work. It should be noted that the results produced were in accordance with the research aim and objectives. Sizing of the columns, reactor, and the cooling system i.e. the cooling jacket were developed from first principle. There has previously been no research carried out on the accurate sizing and flow rate of the cooling medium for the lagging or jacketing of the reactor because HEX reactors have mostly been used for this process. Cooling jackets have mostly been used for processes involving tank reactors such as batch systems or

CSTRs. The lower costs procured from using a cooling jacket to keep the process isothermal against using a heat exchanger tubular reactor is a major economic advantage.

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