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# CSTR Design for Propylene Glycol Chemical Production

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***Abstract*: - The production of propylene glycol chemical from the hydrolysis of propylene oxide in the presence of an acid catalyst in a non-isothermal continuous stirred tank reactor is presented using advanced process simulation software. The steady state design models used in obtaining the reactor parameters such as volume, length, diameter, space time, space velocity were developed by performing material balance over the reactor. The temperature effect was also accounted for using the principle of energy balance over the reactor. The accuracy of the design parameters were ascertained by comparing predicted results with literature data of CSTR for production of propylene glycol. The simulation of the design models were performed using MATLAB. The reactor operates optimally at fractional conversion of 0.9 to obtain optimum values of the most significant variables/parameters [volume of reactor 60.50m$^3$, length of the reactor 6.75m, diameter of reactor 3.37m, space time 2542.02sec, space velocity 0.0004sec$^{-1}$, quantity of heat generated per unit volume of reactor -1.338j/s/m$^3$]. The result obtained from the steady state simulation shows that the feed flow rate, temperature and pressure influence the efficiency of the continuous stirred tank reactor.**

## I. INTRODUCTION

Natural gas is a starting feed material for propylene oxide production in the downstream. Nigeria is ranked sixth largest gas reserves making propylene glycol chemical production local content driven very imperative [21].Propylene glycol is a synthetic liquid.

Propylene glycol group of chemical compounds consist of monopropylene glycol (PG) with IUPAC 1,2-propanediol, Dipropylene glycol (DPG) IUPAC oxybispropanol and Tripropylene glycol (TPG) IUPAC {(1-methyl-1,2-ethanediol)bis(oxy)} propanol. These chemicals are manufactured as co-products and are used commercially in a large variety of applications such as moisturizer in medicines, cosmetics food, toothpaste, shampoo, hair-wash, car wash, sanitizers and antibacterial lotions. They are available as highly purified products, which meet well defined manufacturing and sales specifications[15].

It has a chemical formula of $C_3H_8O_2$ PG is a colorless liquid with slightly sweet taste, it is more viscous than water meaning that if flows slowly like syrup, its melting point is -58$^0$C, its boiling point is 188.2$^0$C, it has specific gravity of 1.036 implies that it is slightly more dense than water, its vapor pressure at normal room temperature is negligible.

Approximately, ***362,873,896kg per year*** of propylene glycol produced worldwide [. This work focuses on the production of PG from the hydrolysis of propylene oxide in the presence of an acid catalyst. Methanol was also introduced to prevent phase-splitting because propylene oxide is not completely soluble in water. The reaction occurs at a temperature not exceeding 324.7k in a single-tank non-isothermal continuous stirred tank reactor which is the most economic method used for propylene glycol production industrially. The reactor feed were introduced through a mechanically and thermodynamically certified pumps at a volumetric flow rate of 0.0238m$^3$/s.

Considerable works have been done on the production of PG and few of them are cited sequentially as follows: Fogler[6]developed models for production of propylene glycol in a CSTR applying adiabatic condition. The reaction operates at a temperature not exceeding 325K. Rensburg et al[13]developed CSTR simu-link model for propylene glycol production. They developed adjustable mass and energy balance models and predicted the behavior of functional parameters for propylene glycol production.

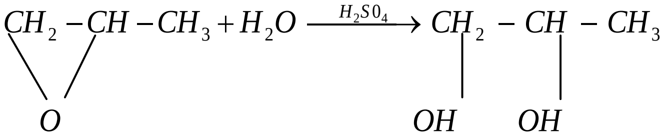
Zahra'a, F. Z[18]focused on the control parameter for a CSTR designed non-isothermally for the production of propylene glycol from the hydrolysis of propylene oxide. The materials used in this work were propylene oxide, water, cooling coil, methanol, stirrer and a CSTR equipment. The work considers the application of energy and material balances including operating conditions and thermodynamic data for the development of the mathematical models used for controlling the process. Arthur & Warren[1]proposed recipe to the manufacture of one batch propylene glycol, they stated that propylene glycol is produced from propylene oxide by liquid phase hydrolysis with excess water in the presence of a small concentration of sulfuric acid as the catalyst. The reaction takes place at a reasonable rate at near ambient temperature, but a temperature rise can be appreciable in a batch reactor.

Piyush & Vyomesh [12]Modeling and simulation of CSTR for manufacture of propylene glycol stated that propylene glycol is produced by direct hydrolysis of propylene oxide with water. They modeled the startup of a CSTR from first principles and simulated using polymath 5.1 and obtained profiles of concentration and temperature.

Base on the economic importance of the petrochemical product in the world, both domestic and industrial applications, the research becomes necessary as it contributes to the growth and development of some countries like China, United State, Russia, India, South Africa and others.

## II. REACTION KINETIC SCHEME

Propylene glycol is produced by the hydrolysis of propylene oxide as shown in the reaction kinetic scheme below.



**[1]**

Equation [1] can be represented hypothetically as;

$$A + B \xrightarrow{K_I} C \qquad [2]$$

Where A = Propylene oxide
B = Process treated water
C = Propylene glycol

The first-order reaction rate [mol/m$^3$/s] with respect to propylene oxide according to[6] can be expressed as;

$$r_A = K_I C_A \qquad [3]$$

Where $r_A$ = Reaction rate and the negative sign implies Depleting rate of the feed (reactant)
$K_I$ = Reaction rate constant (s$^{-1}$)
$C_A$ = Concentration of the species, i.e. propylene oxide

The rate constant temperature dependentfunction according to the Arrhenius equation modelis

$$K_I = A_e^{-E/RT} \qquad [4]$$

Equation [4] was obtained [6]

Combining equation [3] and [4] yields

$$-r_A = Ae^{-E/RT\cdot} C_A \qquad [5]$$

The concentration of propylene oxide ($C_A$) is related to fractional conversion $X_A$ as follows

$$C_A = C_{AO}\left(1 - X_A\right) \qquad [6]$$

Where $C_{AO}$ = Initial concentration of propylene oxide (mol/m$^3$)
$X_A$ = Fractional conversion

Combining equation [5] and [6] yields

$$-r_A = A_e^{-E/RT\cdot} C_{AO}\left(1 - X_A\right) \qquad [7]$$

*2.1 Development of Design Models*

Consider the schematic of one-reactor tank CSTR with feeds and product as shown below.

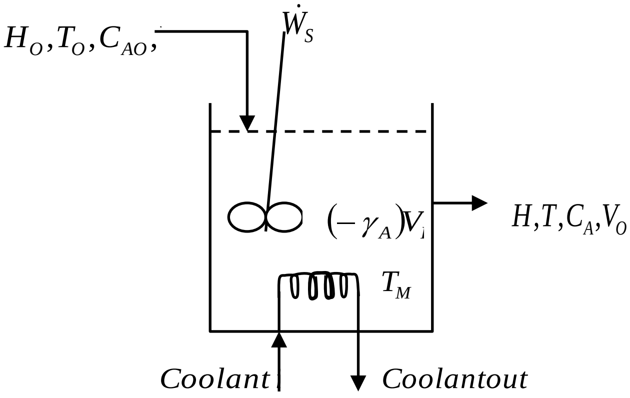


Figure 1 CSTR in Steady State Operation with Heat Effect

The feed stream consists of:

- Propylene oxide
- Sulfuric acid catalyst
- Water

While the product stream is propylene glycol and the unreacted reactant is methanol

*Model Assumptions*

- The feed assumes a uniform composition throughout the reactor.
- The reacting mixture is well stirred.
- The composition of the exit stream is the same as that within the reactor.
- Shaft work by the impeller or the stirrer is negligible.
- The temperature within the reactor is kept at a constant value by the heat exchange medium.

*Volume of the Reactor ($V_R$)*

This can be obtained by applying the principle of material balance stated as follows:

$$\frac{d}{dt}\left(C_A V_R\right) = F_{AO} - \left[F_{AO}\left(1 - X_A\right)\right] - \left(-r_A\right)V_R \qquad [8]$$

At steady state, the accumulation term is equal to zero, i.e.

$$\frac{d}{dt}\left(C_A V_R\right) = 0$$

$$\therefore \quad 0 = F_{AO} - \left[F_{AO}\left(1 - X_A\right)\right] - \left(-r_A\right)V_R \qquad [9]$$

Expanding the bracket

$$0 = F_{AO} - F_{AO} + F_{AO}X_A - (-r_A)V_R$$

$$0 = F_{AO}X_A - (-r_A)V_R$$

$$V_R = \frac{F_{AO}X_A}{(-r_A)} \qquad [10]$$

Substituting equation (7) into equation (10) yields

$$V_R = \frac{F_{AO}X_A}{Ae^{-E/RT}C_{AO}(-r_A)} \qquad [11]$$

*Length of the Reactor ($L_R$)*

Since the reactor is cylindrical, volume of a cylindrical reactor is given as

$$V_R = \pi R^2 L_R \qquad [12]$$

Where:

$V_R$ = Volume of reactor ($m^3$)
R = Radius of reactor (m)
$L_R$ = Length of reactor (m)
π = Constant

Since radius of a cylinder is half its diameter, i.e.

$$R = \frac{D_R}{2} \qquad [13]$$

Where:

$D_R$ = Diameter of Reactor (m).

Combining equation (12) and (13) yields

$$V_R = \pi\left(\frac{D_R}{2}\right)^2 L_R \qquad [14]$$

For a CSTR, the length and diameter ratio is given by [11]

$$\text{Let } \frac{L_R}{D_R} = 2 \qquad [15]$$

$$D_R = \frac{L_R}{2} \qquad [16]$$

Combining equation [14] and [16] yields

$$V_R = \frac{\pi\left(\frac{L_R}{2}\right)^2 L_R}{4}$$

$$V_R = \frac{\pi L^3{}_R}{16}$$

$$\therefore\ L_R = \left(\frac{16V_R}{\pi}\right)^{1/3} \qquad [17]$$

Substituting equation [11] into [2 7] yields

$$L_R = \left[\frac{16\ F_{AO}X_A}{\pi . A_e{}^{-E/RT}C_{AO}\ (1 - X_A)}\right]^{1/3} \qquad [18]$$

*Diameter of the Reactor ($D_R$)*

From equation (16)

$$D_R = \frac{L_R}{2}$$

Substituting equation [18] into [16] yields

$$D_R = \frac{\left[\frac{16\ F_{AO}X_A}{\pi . A_e{}^{-E/RT}C_{AO}\ (1 - X_A)}\right]^{1/3}}{2} \qquad [19]$$

**Space Time [$\tau_{CSTR}$]**

This is defined as the ratio of reactor volume and volumetric flow rate

$$\tau_{CSTR} = \frac{V_R}{v_O} \qquad [20]$$

Substituting equation [11] into [20] yields

$$\tau_{CSTR} = \frac{\frac{F_{AO}X_A}{A_e{}^{-E/RT}C_{AO}\ (1 - X_A)}}{v_O} \qquad [21]$$

$$F_{AO} = C_{AO}v_O \qquad [22]$$

Substituting equation [22] into [21] yields

$$\tau_{CSTR} = \frac{X_A}{A_e{}^{-E/RT}(1 - X_A)} \qquad [23]$$

*Space Velocity ($S_V$)*

This is defined as the reciprocal of space time.

$$S_V = \frac{1}{\tau_{CSTR}} \qquad [24]$$

Substituting equation [23] into [24] yields

$$S_V = \frac{A_e^{-E/RT}\left(1-X_A\right)}{X_A} \qquad [25]$$

### *2.2 Quantity of Heat (Q)*

The quantity of heat generated is mathematically given as

$$Q = \Delta H_R \; F_{AO} X_A \qquad [26]$$

Q = Quantity of heat (J/k)

$\Delta H_R$ = Heat of reaction (KJ/mol)

$F_{AO}$ = Flow Rate of Species (mol/s)

$X_A$ = Fractional Conversion of Species

### *Heat Generated Per Unit Volume of Reactor*

This can be obtained by dividing the quantity of heat generated by the volume of the reactor ($V_R$)

$$\frac{Q}{V_R} = \frac{\Delta H_R \; F_{AO} X_i}{V_R} \qquad [27]$$

$$q = \frac{\Delta H_R \; F_{AO} X_A}{V_R} \qquad [28]$$

Where q = quantity of heat generated per unit volume of the reactor

### *2.3 Energy/Heat Balance*

The energy balance equation is expressed mathematically from first principles as;

$$\rho V_O C_p \frac{dT}{d\tau} = \rho V_O C_p T_o - \rho V_O C_p T - (-r_A) V_R (\Delta H_R) - UA_C (T - T_C) + W_S \qquad [29]$$

**Assumptions**

- Constant density
- System operates at steady state
- Work done by the stirrer is negligible

At steady state,

$$\frac{dH}{d\tau} = \rho C_p V \frac{dT}{dt} = 0$$

Also Neglecting the Shaft Work $W_s$

Equation (29) becomes

$$0 = \rho V_O C_p T_o - \rho V_O C_p T - (-r_A) V_R (\Delta H_R) - UA_C (T - T_C)$$

By rearranging and factorization

$$\rho V_O C_p (T - T_0) = -(-\gamma_A) V_R (\Delta H_R) - UA_C (T - T_C)$$

Dividing through by $\rho V_O C_p$

$$T - T_O = -\frac{(-r_A) V_R (\Delta H_R)}{\rho v_O C_p} - \frac{UA_C (T - T_C)}{\rho v_O C_p} \qquad [30]$$

But $\frac{V_R}{v_O} = \tau \, (space\ time)$

$$T - T_O = \tau \frac{-\Delta H_R r_A}{\rho C_p} - \frac{UA_C (T - T_C)}{\rho v_0 C_p}$$

[31]

Equation (31) can be rearranged to give

$$T = \frac{\tau \; \Delta H_R r_A V_O \; + \; UA_C T_C \; + \; \rho V_O C_P T_O}{\rho V_O C_P \; + \; UA_C} \qquad [32]$$

### *2.4 Reactor Operating Parameters*

The operating parameters of the material and energy balance developed are shown below:

Table 1 shows properties/thermodynamic data

| Data/parameter | Values | Description |
|---|---|---|
| $\rho_A$ | 830kg/m$^3$ | Density of propylene oxide |
| $\rho_B$ | 997kg/m$^3$ | Density of water |
| $\rho_M$ | 792kg/m$^3$ | Density of methanol |
| $\rho_C$ | 1040kg/m$^3$ | Density of propylene glycol |
| $P_O$ | 101325N/m$^2$ | Initial pressure |
| R | 8314Nm mol$^{-1}$ k$^{-1}$ | Gas constant |

Table 2 Calculated Design Data

| Data/parameter | Values | Description |
|---|---|---|
| $M_A$ | 58kg/mol | Molecular weight of propylene oxide |
| $M_B$ | 18kg/mol | Molecular weight of water |
| $M_M$ | 32kg/mol | Molecular weight of methanol |
| $M_C$ | 76kg/mol | Molecular weight of propylene glycol |
| $G_C$ | 14.04kg/s | Mass flow rate of propylene glycol |
| $G_A$ | 10.72kg/s | Mass flow rate of propylene oxide |
| $G_B$ | 3.33kg/s | Mass flow rate of water |
| $G_M$ | 10.72kg/s | Mass flow rate of methanol |
| $\overline{V_A}$ | 0.00121m$^3$/kg | Specific density of propylene oxide |
| $\overline{V_B}$ | 0.001003m$^3$/kg | Specific density of water |

| | | |
|---|---|---|
| $\overline{V}_M$ | 0.001263m$^3$/kg | Specific density of methanol |
| $\overline{V}_C$ | 0.0009621m$^3$/kg | Specific density of propylene glycol |
| $Q_A$ | 0.01297m$^3$/s | Volumetric flow rate of propylene oxide |
| $Q_B$ | 0.01297m$^3$/s | Volumetric flow rate of water |
| $Q_M$ | 0.00757m$^3$/s | Volumetric flow rate of methanol |
| $V_O$ | 0.0238m$^3$/s | Sum of volumetric flow rate of reactants |
| $C_{AO}$ | 0.0424mol/m$^3$ | Initial concentration of propylene oxide |
| $F_{AO}$ | 0.001009mol/s | Initial molar flow rate of propylene oxide |
| $X_A$ | 0.9(dimensionless) | Fractional conversion |
| $\Delta H_R$ | -84666.76j/mol | Change in heat of reaction |
| $\Delta C_P$ | -29.3j/mol k | Change in specific heat capacity |

Table 3 Literature Data with references

| Data | Values | Description | References |
|---|---|---|---|
| $T_O$ | 287.44k | Initial temperature of feed | [Folger, 2006] |
| A | 4.71 x 10$^9$S$^{-1}$ | Pre-exponential factor | [Folger, 2006] |
| E | 75.362kj/mol | Activation energy | [Folger, 2006] |
| T | 324.7k | Operating temperature of the reactor | [Folger, 2006] |
| $H_A$ | -154911.5j/mol | Enthalpy of propylene oxide at 293k | [Rensburg et al., 2013] |
| $H_B$ | -286097.74j/mol | Enthalpy of water at 293k | [Rensburg et al., 2013] |
| $H_C$ | -525676j/mol | Enthalpy of propylene glycol at 293k | [Rensburg et al., 2013] |
| $C_{P_A}$ | 146.5j/mol k | Specific heat capacity of propylene oxide | [Rensburg et al., 2013] |
| $C_{P_B}$ | 75.4j/mol k | Specific heat capacity of water | [Rensburg et al., 2013] |
| $C_{P_C}$ | 192.6j/mol k | Specific heat capacity of propylene glycol | [Rensburg et al., 2013] |
| $T_D$ | 51.67$^0$C | Reactor design temperature | [DOW Chemical Company, 1942] |
| P | 21.7 bar | Reactor design pressure | [DOW Chemical Company, 1942] |

### *2.5 Solution Techniques*

The functional parameters of the reactor and temperature effect models were solved using advanced process simulation software.

*Propylene Glycol Algorithm Simulation Process*

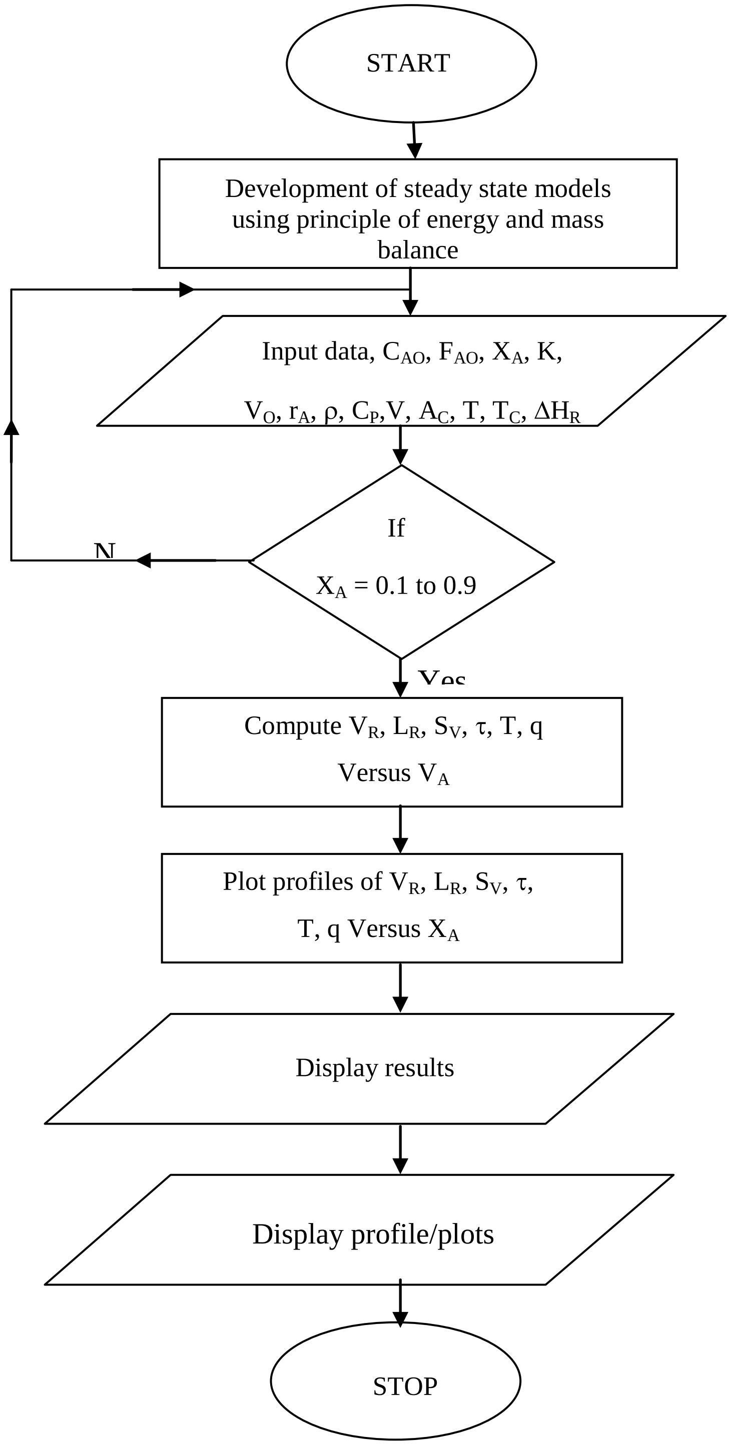


Figure 2 Algorithm of the Simulation Process

## III. RESULTS AND DISCUSSION

The results of the Continuous Stirred Tank Reactor [CSTR] design for the production of ***800 million pounds [362,873,896kg] per year of propylene glycolproduction at 90% fractional conversion*** is presented in table 1 below.

Table 1 Summary of results showing fractional conversion, volume of reactor, length of reactor, space time, space velocity, temperature

1.0e+003 *

| $X_A$ | $V_R$ | $L_R$ | $\tau_{CSTR}$ | $S_V$ | T |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | Inf | 0.2873 |
| 0.0001 | 0.0004 | 0.0012 | 0.0153 | 0.0001 | 0.2873 |
| 0.0001 | 0.0008 | 0.0016 | 0.0322 | 0.0000 | 0.2873 |
| 0.0002 | 0.0012 | 0.0018 | 0.0512 | 0.0000 | 0.2873 |
| 0.0002 | 0.0017 | 0.0021 | 0.0725 | 0.0000 | 0.2873 |
| 0.0003 | 0.0023 | 0.0023 | 0.0966 | 0.0000 | 0.2873 |
| 0.0003 | 0.0030 | 0.0025 | 0.1242 | 0.0000 | 0.2873 |
| 0.0004 | 0.0037 | 0.0027 | 0.1561 | 0.0000 | 0.2874 |
| 0.0004 | 0.0046 | 0.0029 | 0.1932 | 0.0000 | 0.2874 |
| 0.0004 | 0.0056 | 0.0031 | 0.2372 | 0.0000 | 0.2874 |
| 0.0005 | 0.0069 | 0.0033 | 0.2899 | 0.0000 | 0.2874 |
| 0.0005 | 0.0084 | 0.0035 | 0.3543 | 0.0000 | 0.2874 |
| 0.0006 | 0.0103 | 0.0037 | 0.4348 | 0.0000 | 0.2874 |
| 0.0006 | 0.0128 | 0.0040 | 0.5383 | 0.0000 | 0.2874 |
| 0.0007 | 0.0161 | 0.0043 | 0.6763 | 0.0000 | 0.2874 |
| 0.0008 | 0.0207 | 0.0047 | 0.8696 | 0.0000 | 0.2874 |
| 0.0008 | 0.0276 | 0.0052 | 1.1594 | 0.0000 | 0.2874 |
| 0.0008 | 0.0391 | 0.0058 | 1.6425 | 0.0000 | 0.2874 |
| 0.0009 | 0.0605 | 0.0068 | 2.6087 | 0.0000 | 0.2874 |
| 0.0010 | 0.1311 | 0.0087 | 5.5072 | 0.0000 | 0.2874 |

*Reactor Simulation*

The effect of fractional conversion on the following reactor parameters was studied.

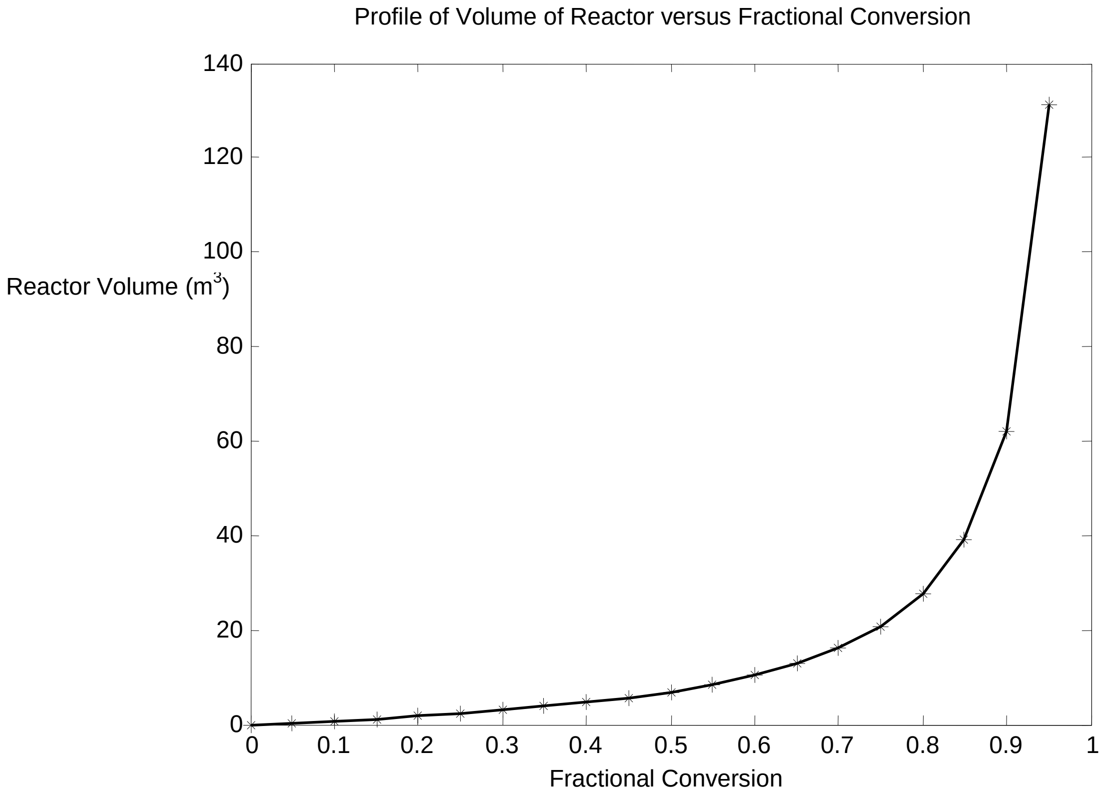


Figure 3: Plots of Reactor Volume against Fractional Conversion

### *3.1 Reactor Volume against Fractional Conversion*

Figure 3 shows the variation of Reactor volume, $m^3$ with fractional conversion, $x_A$ . From the graph, there is an exponential increase in volume with fractional conversion i.e.

$$V \propto e^{x_A}$$

**[33]**

Where K the constant of proportionality takes values from:

O < K < 20, depending on the value of the $x_A$

For instance;

When $x_A$= 0.1, K = 0 and when $x_A = 0.8$, K=20

Hence equation (33) becomes

$$V = ke^{x_A}$$

**[34]**

This implies that the best volume suitable for the process lies between 0.65<$e^{x_A}$<0.9. Higher fraction conversion values say $x_A > 0.85$ give very high volume of the reactor and approaches positive infinity. This is impossible for the system to operates and function optimally. Hence the optimum volume occurs at V = $65m^3$ when the $x_A = 0.88$ shown from the graph in the figure 2 above.

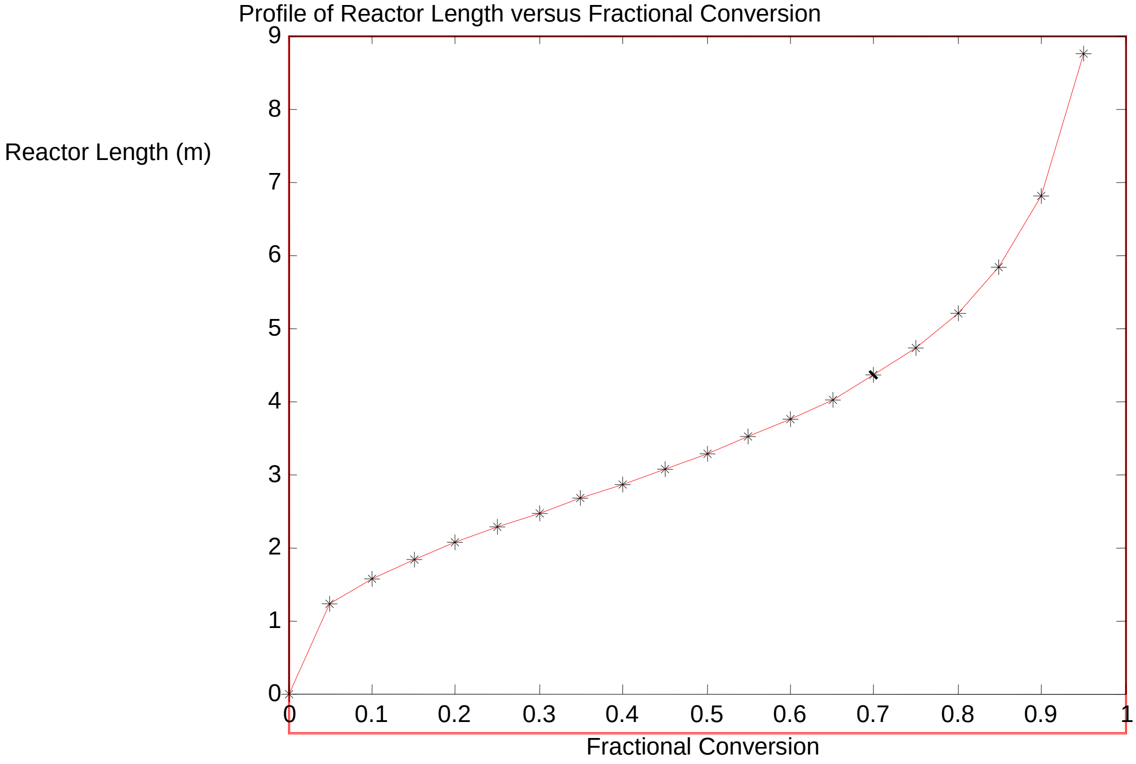


Figure 4: Graph of Reactor Length against Fractional Conversion

### *3.2 Reactor Length against Fractional Conversion*

Figure 4 depicts the variation of reactor length, m with fractional conversion $\boldsymbol{x_A}$ in mol. From the figure, there is progressive increase in reactor length as the fractional conversion increases. It can be shown that, linear increase in reactor length from z=0 to z=1m at $x_A = 0$to $x_A = 0.05$ . Then the increment in length becomes exponential when $\propto_A = 0.05$to $x_A = 0.9$. From this point when $x_A = 0.9,$ higher values of $x_A > 0.9$ causes a very large value for length of the reactor. This proved that the optimal length of the reactor occurs at $x_A = 0.88$, as the $L_{Opt} = 5.5m$.. Thus, the best range of $x_A$ for optimum length of the Reactor to give an optimal yield is at: $0.5 < x_A < 0.88;\ 3m < L < 5.5m$

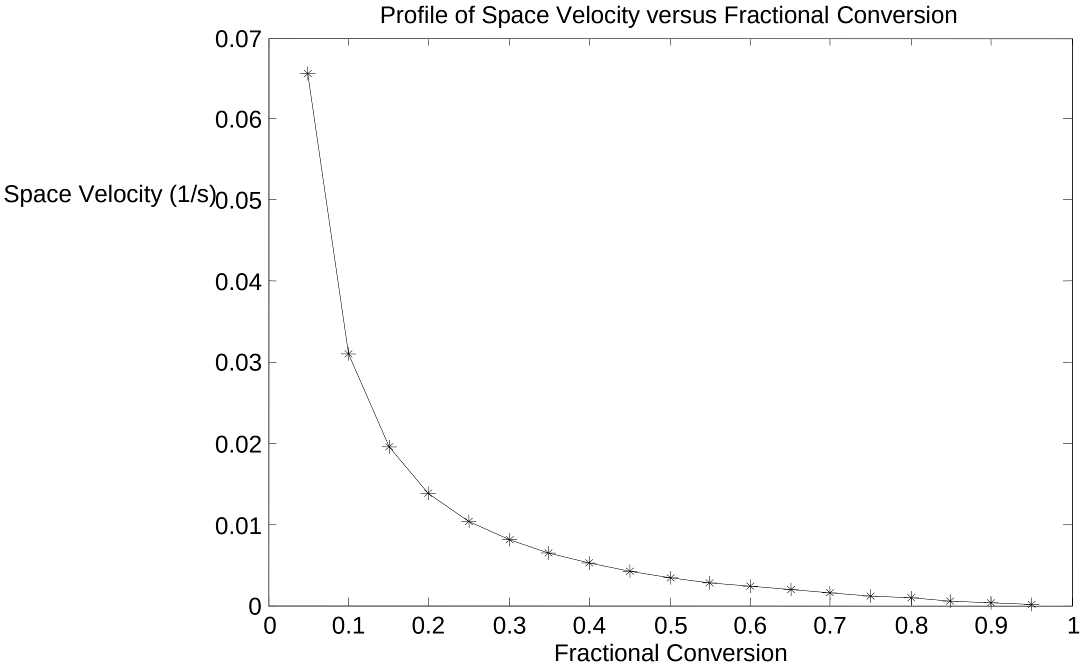


Figure 5: Plots of Space Velocity against Fractional Conversion

*3.3 Space Velocity against Fractional Conversion*

The curve in Figure 5 depicts the relationship of space velocity with fractional conversion. The relationship is inverse exponentially i.e.

$$S_v \alpha e^{-x_A} \quad \textbf{[35]}$$

Smaller value of $x_A$ say 0-0.099 gives very large values of $S_v$ or infinitesimal values of $S_v$ but as fractional conversion, $x_A$ increases from 0.1 to 0.96, the space velocity, $S_v$ decrease exponentially from, $S_v = 0.066s^{-1} to\ S_v = 0s^{-1}$ . This proved that the optimal condition of the CSTR occurs within the range of: $0.45 < x_A < 0.88$

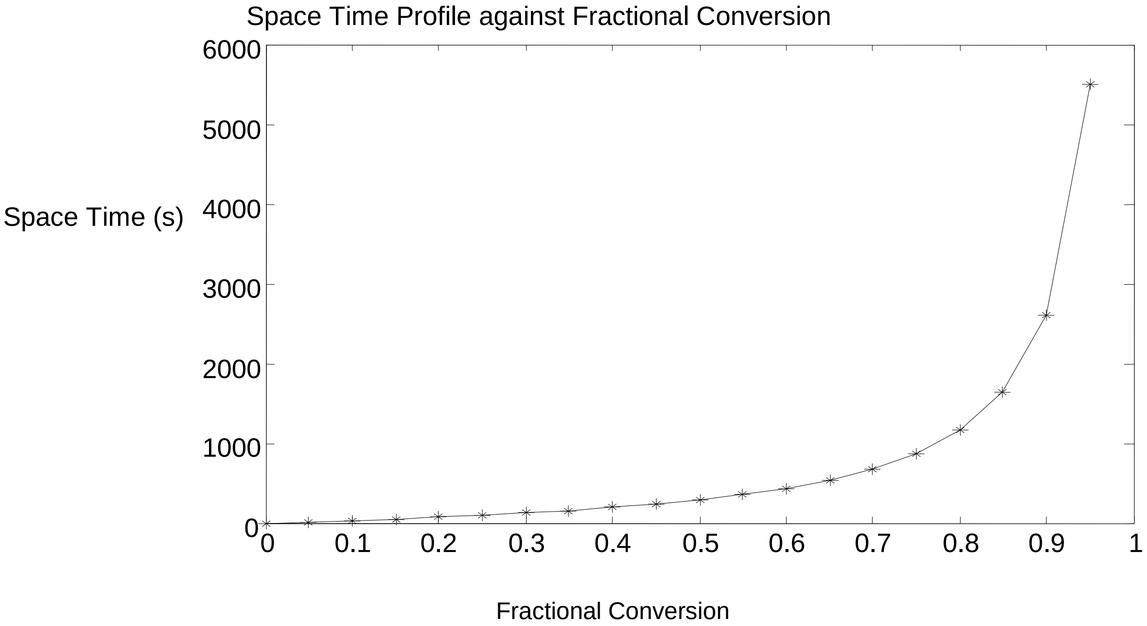


Figure 6: Space Time Variation Profile with Fractional Conversion

### *3.4 Space Time against Fractional Conversion*

Figure 6 shows the variation of space time, $\tau$ with fractional conversion, $x_A$. The variation of $\tau$ increases exponentially with fractional conversion, $x_A$ depending on the proportionally constant from, $x_A = 0$ to $x_A = 0.7$; $\tau$ increase from exponentially from $\tau = 0$ to $\tau = 1000s$. Higher values of fractional conversion increase $\tau$ (space time) to infinitesimal values. Hence, optimal $\boldsymbol{\tau}$ occur when the $x_A = 0.8$. This allows the continuous stirred tank reactor to operate optimally.

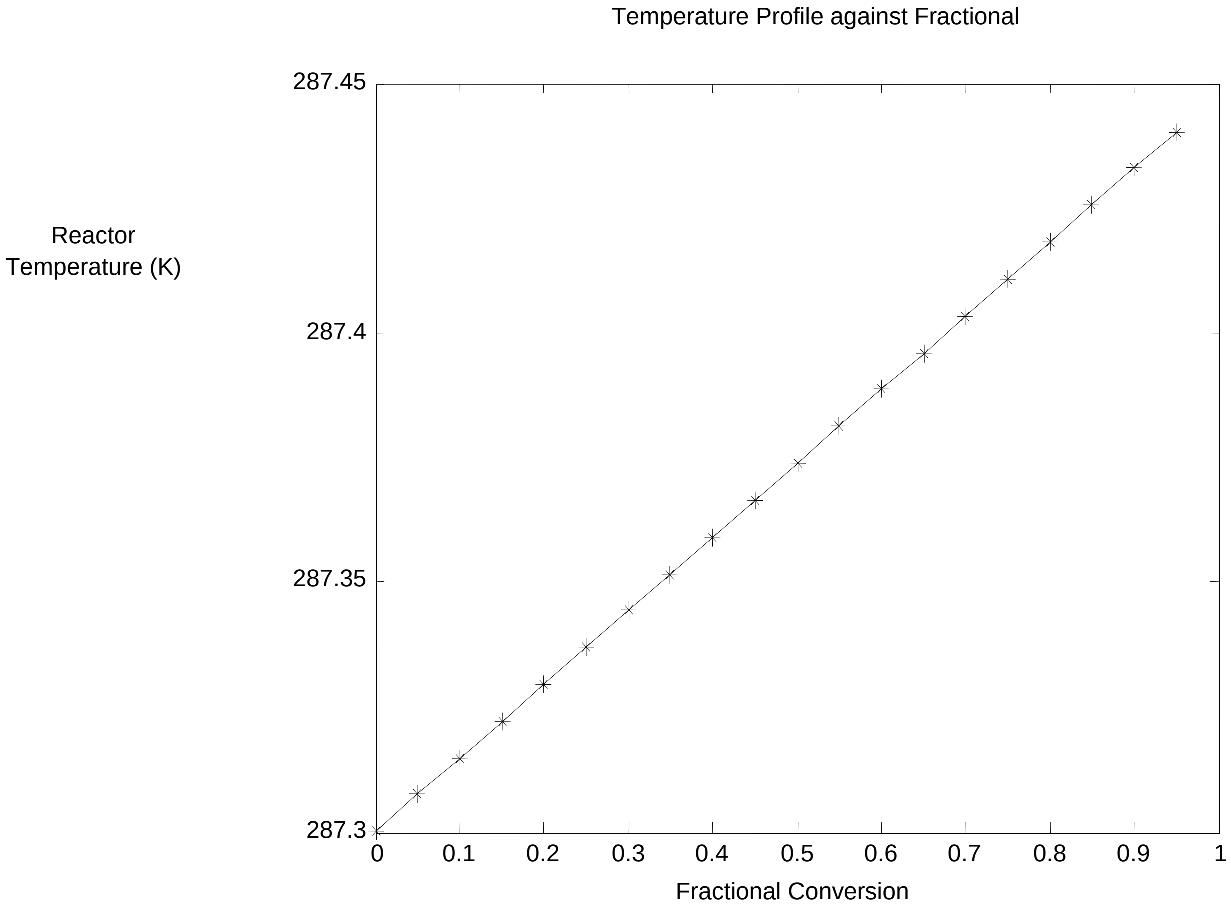


Figure 7 Plots of temperature against fractional conversion

### *3.5 Temperature against Fractional Conversion*

Figure 7 shows the temperature profile with fractional conversion $x_A$. Reactor temperature varies directly and steeply with fractional conversion $x_A$

$T \propto x_A$

**[36]**

This shows that the reaction is endothermic and very little amount of heat is needed for the progress of the reaction. The heat needed for optimum operation is 287.42K and very negligible amount of heat is further added for the reaction process to achieve optimum yield.

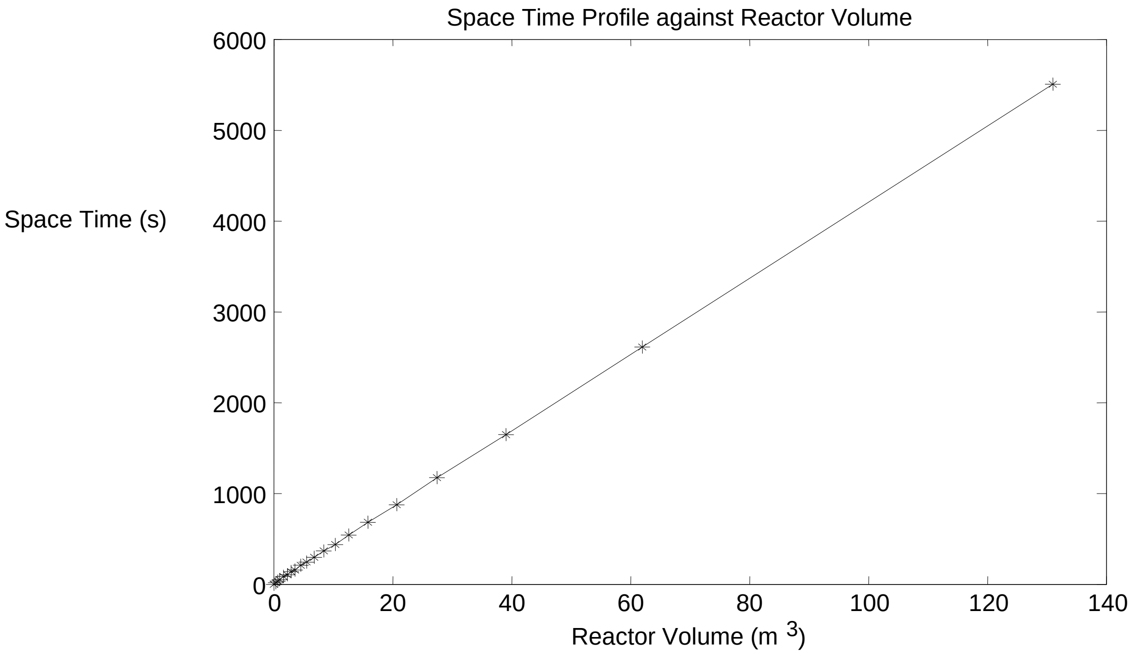


Figure 8 Variation of Space Time with Reactor Volume

*3.6 Space Time versus Reactor Volume*

Figure 8 depicts the variation of space time with reactor volume. The relation is linearly dependent. i.e

$\tau \propto V_R$

**[37]**

Figure 8 indicates that as space time increases, there is a linear increase of reactor volume. From the figure above, the optimal space time value clusters around 0 to 1050s at reactor volume of 0-45m$^3$.

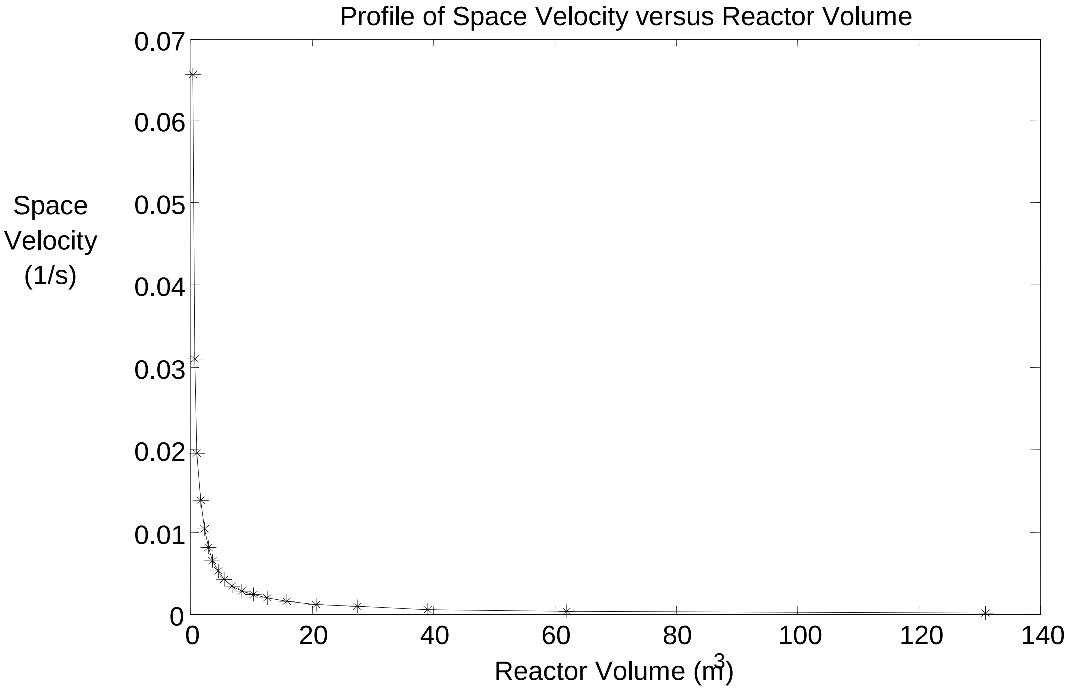


Figure 9: Profile of Space Velocity against Reactor Volume

### *3.7 Space Velocity against Reactor Volume*

Figure 9 shows the graph of space velocity, $S_v$ with reactor volume, $V_R$. that maximum space velocity of $S_v = 0.068\ S^{-1}$ occurs when $V_R = 0m^3$ and exponential drop in $S_v = 0S^{-1}$ at higher values of reactor volume. Thus the optimal yield occurs at very small values of space velocity, $S_v$ for volume of about 60 $m^3$.

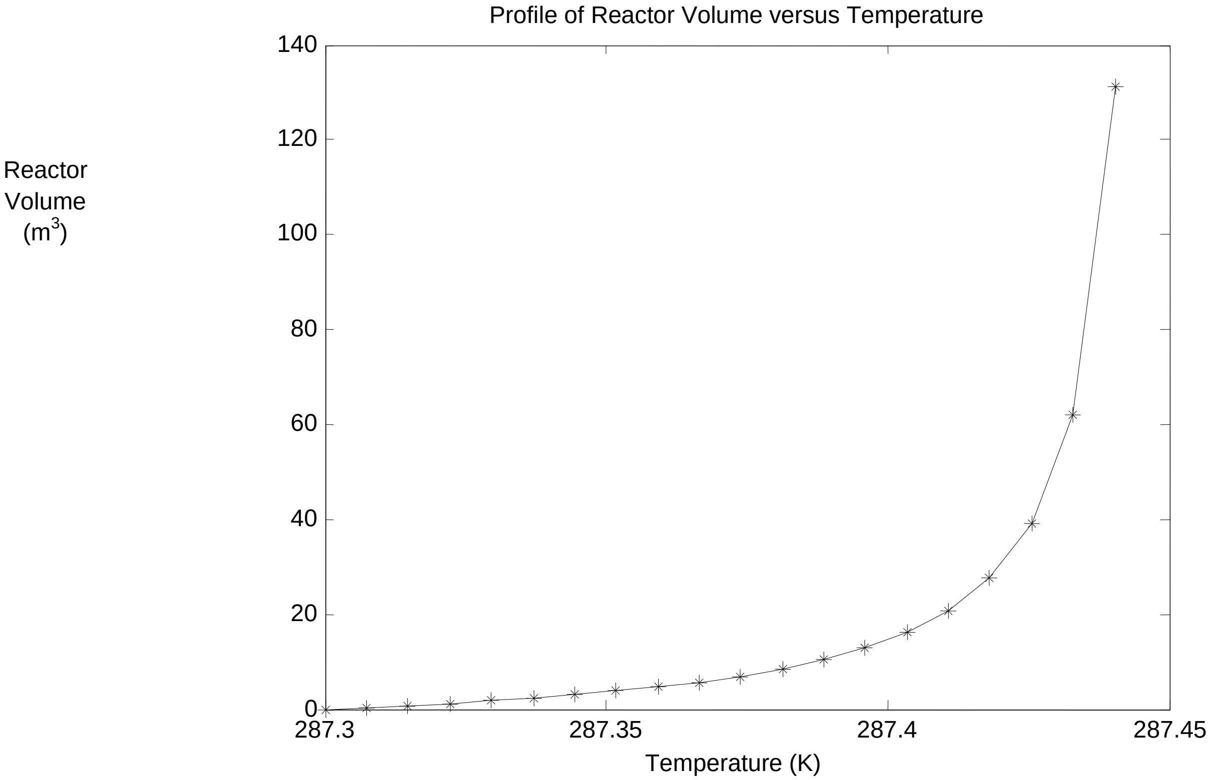


Figure 10: Graph of Reactor Volume against Temperature

### *3.8 Reactor Volume against Temperature*

Figure 10 depicts profile of reactor volume, $m^3$ against temperature K.

From the plot, the volume of the reactor varies exponentially with temperature of the reactor.

$$V \propto e^T \quad \textbf{[38]}$$

When the volume of the reactor is $0m^3$ the temperature increases, the volume of the reactor increases, the volume of the reactor increases exponentially to a point where at T = 287.4k, the volume becomes very large and approaches positive infinity; $V = +\infty$. Hence a reasonable volume say $V = 0m^3$ to $V = 60m^3$ can be when the temperature range is $287.3k < T < 287.42k$.

## IV. CONCLUSION

The research explores ways Nigerian local content Act 2004 can be encouraged in engineering practice.

The aim of this research is to produce 800 million pounds/year of propylene glycol using the hydrolysis of propylene oxide in the presence of an acid catalyst. Methanol was introduced to prevent phase-splitting. The reaction occurs at temperature not exceeding 325K. In a single-tank non-isothermal continuous stirred tank reactor. Which is the most economic method used for propylene glycol production industrially.

The model equations used in obtaining the reactor parameters such as volume, length, diameter, space time, space velocity were developed by performing material balance over the reactor. The temperature effect was also accounted for using the principle of energy balance over the reactor.

The reactor was also optimized in order to obtain optimum reactor parameters and operating conditions. Mechanical design was also carried out to determine which material type of reactor will be most economically suitable for optimum production thereby maximizing profit. Some of the reactor parameters were simulated using MATLAB program to allow variable parameters to be used in testing the models and to ensure flexibility.

The MATLAB simulated results are summarized in Table 4.2 and profiles of the simulations are shown in Figures 4.1 to 4.7. The discussions of the profiles plotted were in agreement with the objectives of this thesis.

## NOMENCLATURE

| Symbol | Definition | Units |
|---|---|---|
| $M_A$ | Molecular weight of propylene oxide | $Kg/mol$ |
| $M_B$ | Molecular weight of water | $Kg/mol$ |
| $M_M$ | Molecular weight of methanol | $Kg/mol$ |
| $M_C$ | Molecular weight of propylene glycol | $Kg/mol$ |
| $G_C$ | Mass flow rate of propylene glycol | $Kg/S$ |
| $G_A$ | Mass flow rate of propylene oxide | $Kg/S$ |
| $G_B$ | Mass flow rate of water | $Kg/S$ |
| $G_M$ | Mass flow rate of methanol | $Kg/S$ |
| $\rho_A$ | Density of propylene oxide | $Kg/m^3$ |
| $\rho_B$ | Density of water | $Kg/m^3$ |
| $\rho_C$ | Density of propylene glycol | $Kg/m^3$ |
| $\rho_M$ | Density of methanol | $Kg/m^3$ |
| $\bar{v}_A$ | Specific density of propylene oxide | $m^3/kg$ |
| $\bar{v}_B$ | Specific density of water | $m^3/kg$ |
| $\bar{v}_C$ | Specific density or propylene glycol | $m^3/kg$ |
| $\bar{v}_M$ | Specific density of methanol | $m^3/kg$ |
| $Q_A$ | Volumetric flow rate of propylene oxide | $m^3/S$ |
| $Q_B$ | Volumetric flow rate of water | $m^3/S$ |
| $Q_M$ | Volumetric flow rate of methanol | $m^3/S$ |
| $V_O$ | Total volumetric flow rate of reactants | $m^3/S$ |
| $C_{AO}$ | Initial concentration of propylene oxide | $mol/m^3$ |
| $[_{AO}$ | Initial molar flow rate of propylene oxide | $mol/m^3$ |
| $P_O$ | Initial pressure of feed | $N/m^2$ |
| $T_O$ | Initial temperature of feed | Kelvin |
| A | Frequency factor | $S^{-1}$ |
| E | Activation energy | $Kj/mol$ |
| $K_I$ | Rate constant of reaction | $S^{-1}$ |
| $r_A$ | Reaction rate | $mol/m^3/s$ |
| $X_A$ | Fractional conversion | Dimensionless |
| $V_R$ | Volume of reactor | $m^3$ |
| $L_R$ | Length of reactor | m |
| $D_R$ | Diameter of reactor | m |
| $S_V$ | Space velocity | $S^{-1}$ |
| Q | Quantity of Heat | j/s |
| q | Quantity of Heat per unit volume of reactor | $j/s.m^3$ |
| $T_C$ | Coolant temperature | K |
| $C_{P_A}$ | Specific heat capacity of propylene oxide | j/mol k |
| $C_{P_B}$ | Specific heat capacity of water | j/mol k |
| $C_{P_C}$ | Specific heat capacity of propylene glycol | j/mol k |
| $\Delta C_P$ | Change in specific heat capacity | j/mol k |
| $H_A^O$ | Enthalpy of propylene oxide | j/mol |
| $H_B^O$ | Enthalpy of water | j/mol |
| $H_C^O$ | Enthalpy of propylene glycol | j/mol |
| $\Delta H_R$ | Change in enthalpy of reaction | j/mol |

$\rho$ = Density of Liquid in the tank ($kg/m^3$)
$V_R$ = Volume of Reactor ($m^3$)
$C_p$ = Specific Heat Capacity of Material (KJ/kmol.K)
T = Operating Temperature of the Medium (K)
$\tau$ = Space Time (sec)
$V_O$ = Volumetric Flow Rate ($m^3/s$)
$(-r_A)$ = Reaction Rate ($mol/m^3/s$)
$(\Delta H_R)$ = Heat of Reaction (KJ/mol)
U = Coefficient of Heat Transfer
$A_c$ = Area of the coolant ($m^3$)
A = Pre-exponential factor or frequency factor (/s)
E = Activation Energy (J/mol.s)
R = Gas Constant (J/mol/k)

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