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Plant Design for the Production of 2-Ethylhexanol from Propylene and Synthesis Gas

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Abstract **Original Research Article**

The design of a plant for the production of 72,000 tonnes per year of 2-ethylhexanol was considered in this work. The unit operations considered in the plant was separator; reactor and distillation column, the design models for the separator, plug flow reactor and distillation column are presented. The process flow diagram showing the unit operations was designed and simulated with Aspen Hysys and MS Excel used for the plotting of results. The plug flow reactor was designed with fractional conversion, x_A = 0.99 for volume of reactor = 2.5 x 10^{-5} m^3, diameter of reactor = 0.02539m, length of reactor = 0.05078m, space time = 5.76 x 10^{-6}hr, space velocity = 173711.6hr^{-1}, heat generated per unit volume = -5.61 x10^6KJ and pressure drop = 2.61 x 10^{-10}Pa. Diameter of distillation column = 1.473192m, distillation column down comer area = 0.204545 m^2 and distillation column weir length = 1.119626m while separator had the following parameter; area of packed bed column = 4.440853m^2, diameter = 2.377871m and height = 31.66393m. The values of a design parameters of the plug flow reactor, distillation column and separator showed optimum results and reliable based on standard specification.

Keywords: Reactor, distillation column, 2-ethylhexanol, Propylene, Synthesis gas.

1.0 INTRODUCTION

2-ethylhexanol is applicable as a feedstock in the production of plasticizers and lubricants, where it is used as a precursor for the synthesis and because it is a fatty alcohol, its esters tend to have emollient properties. It is also use as low volatile solvent and octane booster when reacted with nitric acid. It aids the production of glycidyl which is use as a coatings, adhesives and sealants application. The production of 2-ethylhexanol has several applications, and hence the design of plant for its production will be of benefit for any economy. 2-ethylhexanol is an alcohol with eight-carbon branches. It is a colourless liquid that has low solubility in water but more soluble in organic solvents. It is industrially produced on a large scale of about 2,000,000,000 kg/year base on its several industrial applications [1]. It was reported that 2-ethylhexanol is produced by the aldol condensation on butyraldehyde followed by hydrogenation of the resulting hydroxyaldehyde. About 2,500,000 tonnes are prepared from this process yearly [2]. Research has now shown that new methods for the production of 2-ethylhexanol is been studied [2]. Also, the unit operations in the plant will be sized or design such that the production will be in excess to meet current demand of world's population as at 2019.

The design of plant for the production of 72,000 tonnes per year of 2-ethylhexanol from propylene and synthesis gas is proposed to generate excess of it to the world's population today. It was reported that 2,000,000,000 kg/yr of 2-ethylhexanol was produced. This rate was suitable as at that time but not in excess to accommodate the demand for today. For this reason, as the year increases, the world's population increases and the demand for the said product base on its application in process industries has increased as well.

To this ends, there is inadequacy in the supply and production of 2-ethylhexanol to the world's industrialization. New methods and areas of applications are been discovered. The research for how to produce more is still on and the process continuous. This research has been of great interest as to design a plant for the production of 2-ethylhexanol that will meet the requirement of the world's industrialization today and even have excess of the product for reserve for more than a decade.

2.0 MATERIALS AND METHODS

2.1 General Material Balance Equation

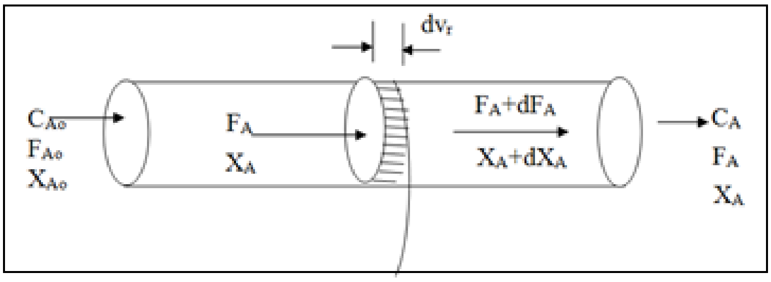


Fig-1: Schematic Diagram for a Plug Flow

The design performance equations for the rector and separators were developed by the application of the principles of conservation of mass given in equation 1.

$$\begin{pmatrix} Rate\ of\ accumulation \\ of\ component\ i \\ wihtin\ the\ reactor \end{pmatrix} = \begin{pmatrix} Rate\ of\ input \\ of\ component \\ i \end{pmatrix} - \begin{pmatrix} Rate\ of\ output \\ of\ component \\ i \end{pmatrix} \pm \begin{pmatrix} Rate\ of\ generation\ or \\ deplection\ of\ species\ i \\ by\ chemical\ reactor \end{pmatrix} \quad (1)$$

2.2.1 Material Balance over the Column

Molar Flow rate of Feed

The product from the pump is given in terms of volumetric flow rate, so it will be converted to molar flow rate using the below formula:

Mass flow rate = density * volumetric flow rate

Molar flow rate = $\frac{Mass\ flow\ rate}{molar\ mass}$ (2)

$$F = \frac{\rho_{mix}}{M} V_o \quad (3)$$

$$\rho_{mix} = x_{fB}\rho_B + x_{fM}\rho_M + x_{fD}\rho_D \quad (4)$$

$$M = x_{fB}M_B + x_{fM}M_M + x_{fD}M_D \quad (5)$$

Determination of Distillate and Bottoms Flowrates

Making reference to chemical engineering design textbook

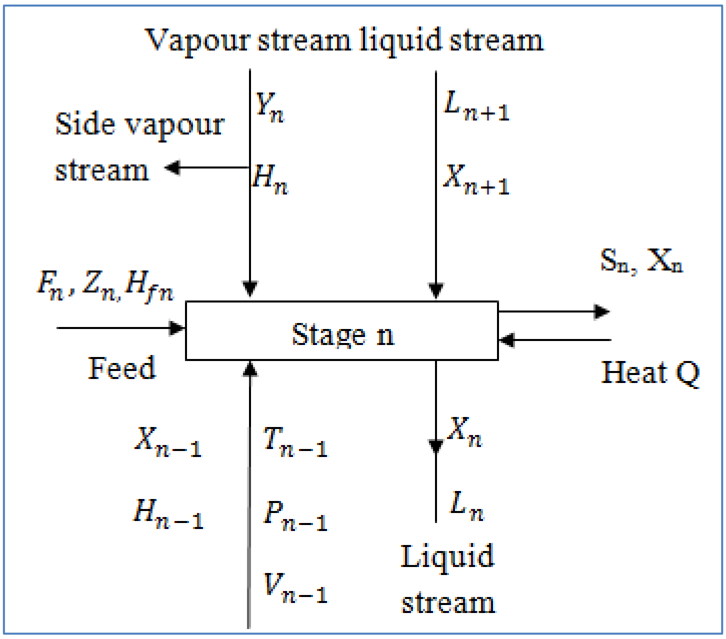


Fig-2: Multi Component distillation Column Diagram for Stage n (feed)

Substituting the assumptions for the distillation column into the general material balance equation as shown in equation 1, we obtained;

$$\begin{pmatrix} Rate\ of\ input \\ of\ component \\ i \end{pmatrix} = \begin{pmatrix} Rate\ of\ output \\ of\ component \\ i \end{pmatrix} \quad (6)$$

Taking overall balance around the column

F = D - B (7)

From equation (7)

B = D - F (8)

Taking component balance with respect to benzene (B)

$$x_{fB}F = y_B D + x_{BB} B \quad (9)$$

Putting (8) into (9)

$$x_{fB}F = y_B D + x_{BB}(\mathrm{D} - \mathrm{F}) \quad (10)$$

Simplifying equation (10) and making D the subject of formula we have;

$$D = F(\frac{x_{fB}+x_{BB}}{y_B-x_{BB}}) \quad (11)$$

Taking balance around the condenser

$$V_n = L_n + D \quad (12)$$

But:

$$R = \frac{L_n}{D} \quad (13)$$

From equation (13)

$$L_n = R \times D \quad (14)$$

Determination of Upper and Lower Operating Line Equation

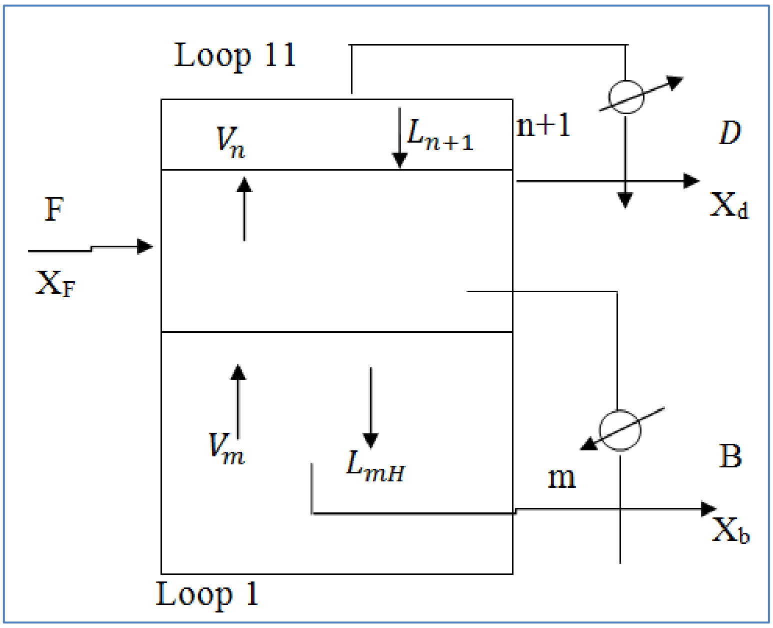


Fig-3: Schematic Diagram of Distillation Column

The upper operating line equation as proposed by Lewis – Sorel is given as;

$$Y_n = \frac{L_n}{L_n+D} x_n + \frac{D}{L_n+D} x_d \quad (15)$$

Similarly, the lower operating line equation is given by;

$$Y_m = \frac{L_m}{V_m} x_m + \frac{W}{V_m} x_{BB} \quad (16)$$

Determination of Column Pressure Drop

$Column\ pressure\ drop\ per\ plate = \rho gh * No.of\ stages$ (17)

But;

$\Delta P = P_B + P_T$ (18)

Where: P_B is the pressure at bottom of column

P_T is the pressure at the top of the column

Determination of Column Diameter

The column diameter will be obtained from the column area Ac which is a function of the net area A_N of the column.

$A_N = 88\%\ of\ A_C$ (19)

From equation (19)

$A_C = \frac{A_N}{0.88}$ (20)

But, $A_N = \frac{Maximum\ Volumetric\ flowrate}{Average\ Vapour\ Velocity}$ (21)

Mathematically;

$A_N = \frac{U_V}{U_n}$ (22)

Where; $U_n = \%flooding * flooding\ velocity(U_f)$ (23)

Before we can calculate the flooding velocity, we need to determine the column liquid vapour flowrate F_{LV}

At the top: $F_{LV} = \frac{L_n}{V_n}\sqrt{\frac{\rho_v}{\rho_L}}$ (24)

At the bottom: $F_{LV} = \frac{L_m}{V_m}\sqrt{\frac{\rho_v}{\rho_L}}$ (25)

The flooding velocity U_f is calculated using;

$U_f = k_1\sqrt{\frac{\rho_L-\rho_v}{\rho_v}}$ (26)

The average vapours velocity for design of 80% flooding

At Top: $U_n = U_f * 0.8$ (27)

At Bottom: $U_n = U_f * 0.8$ (28)

The maximum volumetric flow rate $\dot{U}$

$\dot{U} = \frac{V*M}{\rho_v*3600}$ (29)

Hence, the net area A_N is given for both top and bottom as;

$A_N = \frac{\dot{U}}{U_n}$ (30)

Assuming the column to be cylindrical; area of a cylinder is given by;

$A_C = \frac{\pi {D_c}^2}{4}$ (31)

Making the diameter the subject of formula of equation (3.52)

$D_C = \sqrt{\frac{4A_C}{\pi}}$ (32)

Equation (3.53) is used to calculate the diameter for the top and bottom part of the column.

Determination of Height of Column

$Height\ of\ column = No.of\ stages * Tray\ spacing$ (33)

Design of Sieve Plate for the Column

Area of Column Ac

$$Ac = \frac{\overline{\wedge} D_c^2}{4}$$

Down comer Area

$$A_d = \frac{12}{100} A_c \quad (34)$$

Active Area

$$A_a = A_C - 2A_d \quad (35)$$

Hole Area

$$A_h = 0.1A_C \quad (36)$$

Weir length

$$L_w = 0.1D_C$$

Weir heightL_w = 50mm (atmosphere Distillation)

Hole diameterD_h = 5mm

Plate thickness = 5mm (carbon in steel)

$$\text{Number of holes on plate} = \frac{\textit{Hole Area}}{\textit{Area of one hole}} \quad (37)$$

$$\text{Area of one hole } A_h = \frac{\pi d_h^2}{4} \quad (38)$$

Determination of hole pitch (Distance between two holes)

$$\textit{Area of perforation Ap} = \textit{Active Area} - \textit{Area of unperforated edge} - \textit{Area of calming Zone} \quad (39)$$

Mathematically,

$$A_p = A_A - A_{up} - A_{cz} \quad (40)$$

But,

$$A_{up} = L_{up} * W_{up} \quad (41)$$

$$L_{up} = \left(D_C - W_{up}\right)\pi * \left(\frac{180-\theta_C}{180}\right) \quad (42)$$

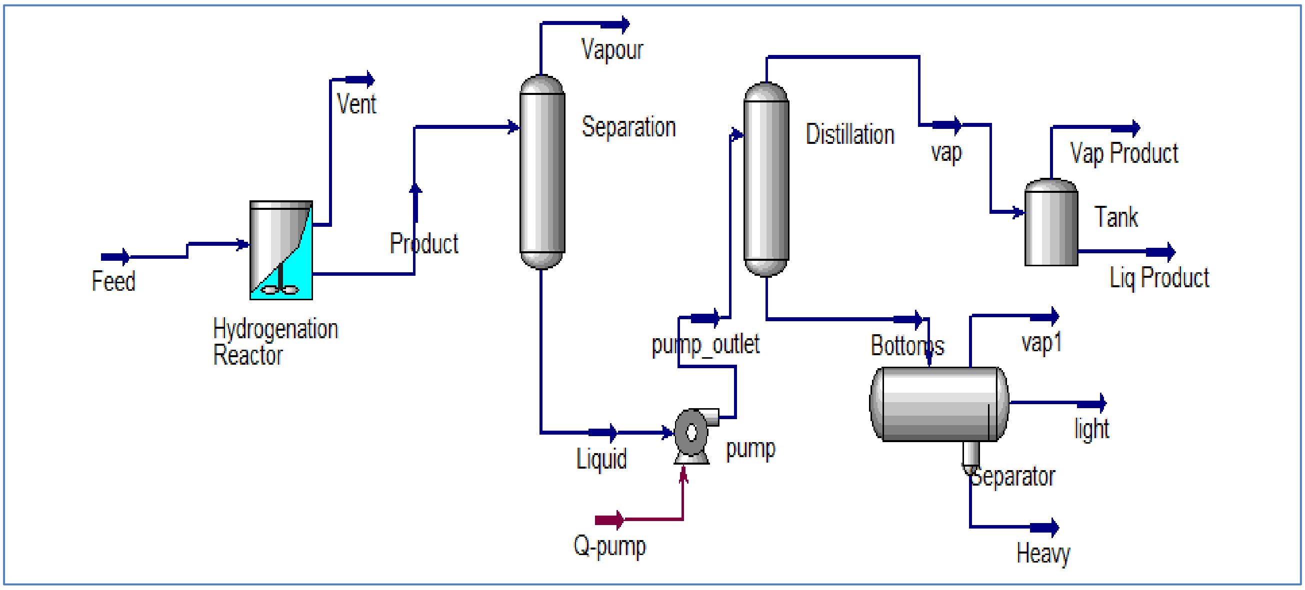
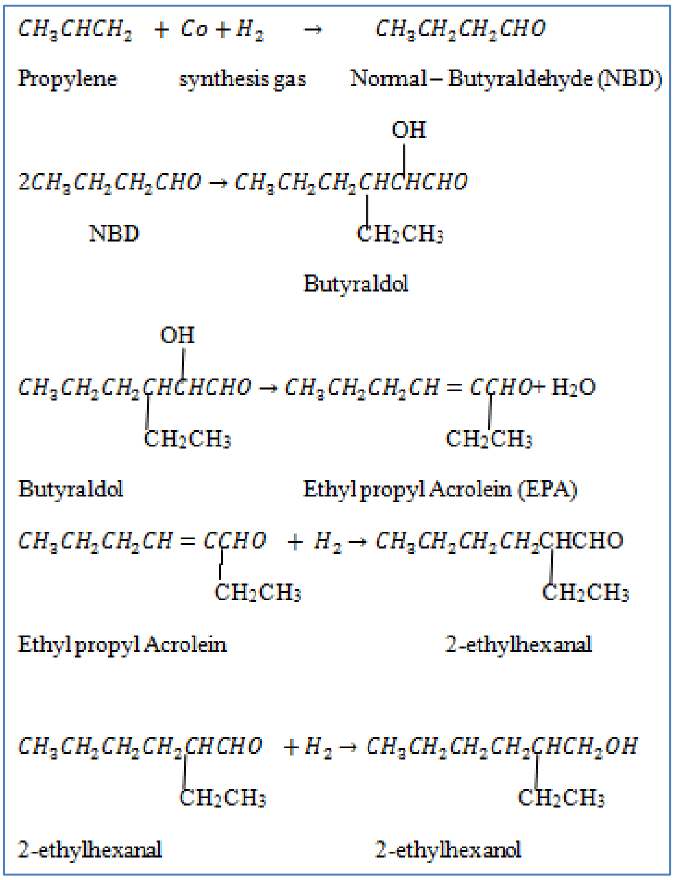


Fig-4: Aspen Hysys Simulation of the Plant

Determination of rate Expression

The production of 2-ethylhexanol is based on the reaction of synthesis gas and propylene as reactants. The reaction mechanism is as follows:



Kinetics of the Reaction

If the reaction takes place on 1:1 Hydrogen to carbon monoxide ratio, the rate will be independent of total pressure, since the rate law is proportional to hydrogen and inversely proportional to carbon monoxide.

Hence, the reaction rates in the temperature range 110-118^{0}c require high carbon monoxide partial pressure (PCO) and total H_2/CO pressure of 200-300 bar.

The rate of reaction is

$$\frac{d}{dt}(aldehyde) = K_{obs}[Alkene][H_2][C_o][Co]^{-1}$$

$$(-r_A) = \frac{K_{obs}[Alkene][H_2][C_o]}{[Co]} \quad (43)$$

4.0 RESULTS AND DISCUSSION

4.1 Results

The models for the design parameters of the reactor, distillation column and packed bed column were presented in chapter 3. The simulation of the model was done using a computer program writing with MATLAB and SIMULINK compiler.

Table-1: Results of simulation of Design Parameters of reactors

Fractional conversion %	Vr (m^3)	Dr(m)	Lr(hr)	St(hr)	Sv(hr^{-1})	Qr(m^{-3})	DP(bar)
0.20	1.25E-06	0.009256	0.018513	2.79E-07	3.59E+06	-2.34E+07	3.61E-10
0.40	2.85E-06	0.0122	0.024399	6.39E-07	1.57E+06	-2.04E+07	3.30E-10
0.60	5.12E-06	0.014823	0.029646	1.15E-06	8.73E+05	-1.71E+07	3.10E-10
0.80	8.99E-06	0.017884	0.035769	2.01E-06	4.97E+05	-1.30E+07	2.92E-10
0.99	2.57E-05	0.02539	0.05078	5.76E-06	173711.6	-5.61E+06	2.61E-10

Table-2: Results of simulation of design Parameters of distillation column

Ac(m^2)	Dc(m)	Ad(m^2)	An(m^2)	Aa(m^2)	Lw(m)
0.568182	0.850548	0.068182	0.5	0.431818	0.646416
1.136364	1.202856	0.136364	1	0.863636	0.914171
1.704545	1.473192	0.204545	1.5	1.295455	1.119626
2.272727	1.701096	0.272727	2	1.727273	1.292833
2.840909	1.901883	0.340909	2.5	2.159091	1.445431

Table-3: Table 42: Results of simulation of design Parameters of packed bed column

Molar flowrate (kgmole/h)	Acp(m^2)	Dcp(m)	Hog(m)
6.87	4.440853	2.377871	31.66393
7.63	4.932127	2.505949	33.7427
8.93	5.772463	2.711038	37.29848
9.73	6.289593	2.829869	39.48665
10.52	6.800259	2.942509	41.64747

However, the reactor was simulated by varying the fractional conversion. The design parameters of the distillation column varying with net area. The design parameters varying with mass flow rate of the packed bed column.

4.2 DISCUSSION

The design parameters of the reactor, distillation column and packed bed column are simulated by varying sensitive parameters of each unit operations. The various unit operations will be discussed with respect to the design parameters.

4.2.1 Effect of fractional conversion with Volume of reactor

From Figure 2, the graph below shows the variation of fraction conversion with volume of reactor.

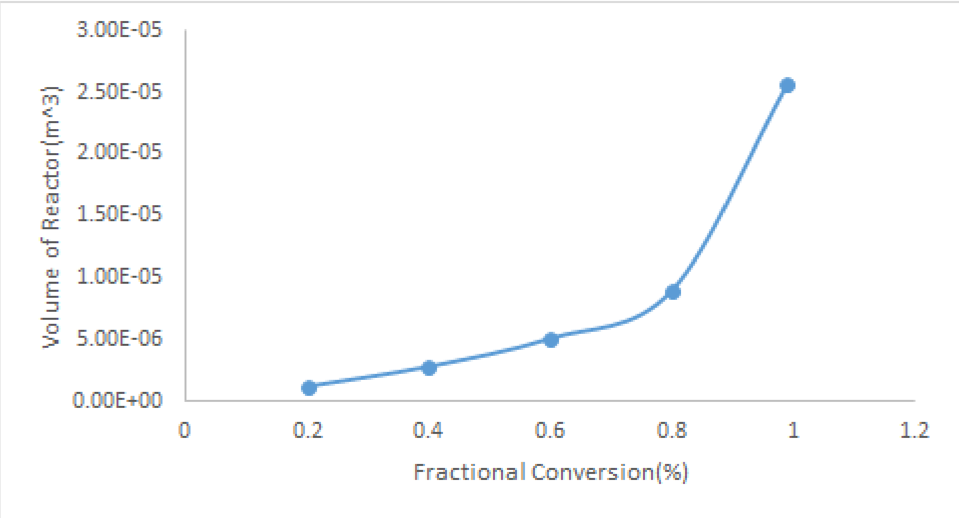


Fig-2: Effect of Fractional Conversion with Volume of Reactor

The fractional conversion has an effect on the volume of the reactor by increasing the volume of the reactor has fractional conversion increase. The fractional conversion which started from 0.02 causes the volume of reactor to increase till it attains a maximum volume of about 0.00005. The increase of the volume of reactor causes an increase in the fractional conversion which increases the rate of production in the reactor.

However, as the fractional conversion increase, the volume of the reactor increases, the diameter became maximum as fractional conversion increases to X_A = 0.99. Hence, the cause of increase in the fractional conversion which causes increase in the volume of reactor makes the graph to be upward slope graph (curve).

4.2.2 Effect of Fractional Conversion with Diameter of Reactor

From Figure 3, the graph below shows the variation of fractional conversion with diameter of reactor.

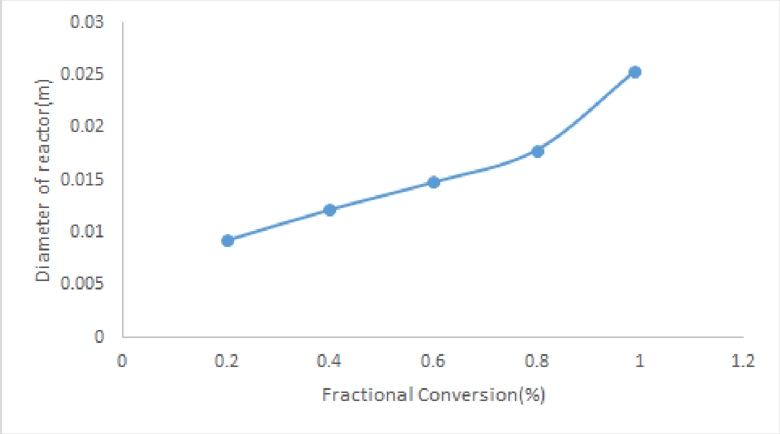


Fig-3: Effect of Fractional Conversion with Diameter of Reactor

The fractional conversion has an effect on the diameter of the reactor by increasing the diameter of the reactor has fractional conversion increase. The fractional conversion which started from 0.02 causes the diameter of reactor to increase till it attains a maximum diameter of about 0.03. The increase of the diameter of reactor causes an increase in the fractional conversion which increases the rate of production in the reactor.

However, as the fractional conversion increase, the diameter of the reactor increases, the diameter became maximum as fractional conversion increases to X_A = 0.99. Hence, the cause of increase in the fractional conversion which causes increase in the diameter of reactor makes the graph to be upward slope graph (curve).

4.2.3 Effect of Fractional Conversion with Length of Reactor

From Figure 4, the graph below shows the variation of fractional conversion with length of reactor.

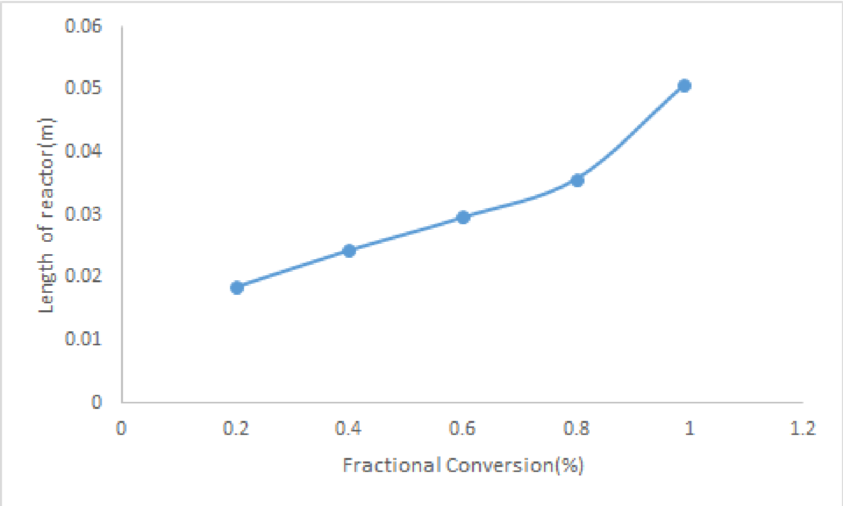


Fig-4: Effect of Fractional Conversion with Length of Reactor

The fractional conversion has an effect on the length of the reactor by increasing the length of the reactor has fractional conversion increase. The fractional conversion which started from 0.02 causes the length of reactor to increase till it attains a maximum length of about 0.05. The increase of the length of reactor causes an increase in the fractional conversion which increases the rate of production in the length.

However, as the fractional conversion increase, the length of the reactor increases, the length became maximum as fractional conversion increases to X_A = 0.99. Hence, the cause of increase in the fractional conversion which causes increase in the length of reactor makes the graph to be upward slope graph (curve).

4.2.4Effect of Fractional Conversion on Space Time

From Figure 5, the graph below shows the variation of fractional conversion with respect to space time.

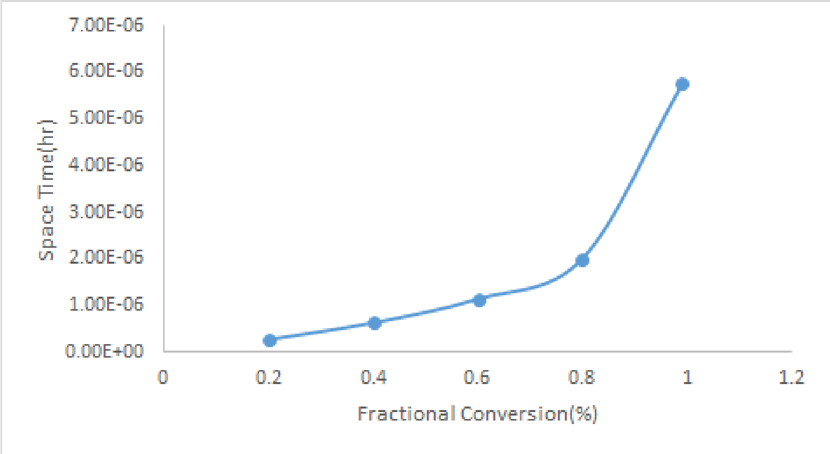


Fig-5: Effect of Fractional Conversion with Space Time

The fractional conversion has an effect on the space time of the reactor by increasing the space time of the reactor has fractional conversion increase. The fractional conversion which started from 0.02 causes the space time of reactor to increase till it attains a maximum space time of about 0.000005. The increase of the space time of reactor causes an increase in the fractional conversion which increases the rate of production in the space time.

However, as the fractional conversion increase, the space time of the reactor increases, the space time became maximum as fractional conversion increases to X_A = 0.99. Hence, the cause of increase in the fractional conversion which causes increase in the space time of reactor makes the graph to be upward slope graph (curve).

4.2.5Effect of Fractional Conversion of Space Velocity

From Figure 6, the graph below shows the variation of fractional conversion on space velocity.

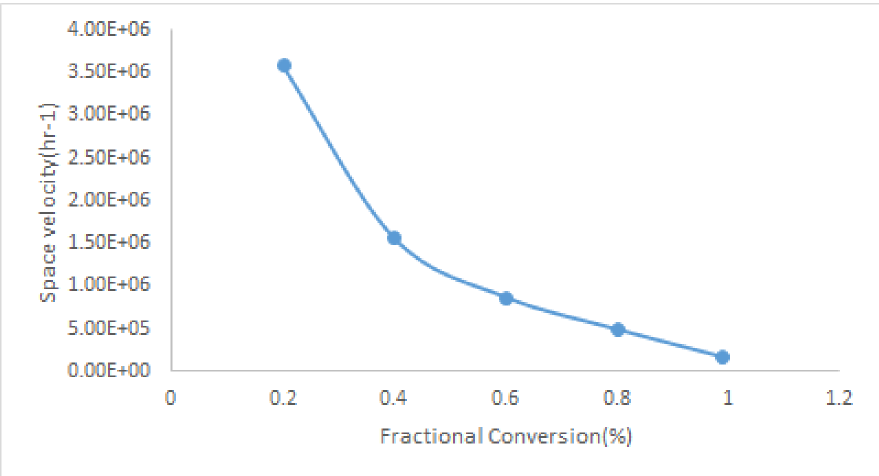


Fig-6: Effect of Fractional Conversion on Space Velocity

The fractional conversion causes a negative effect on the space velocity by causing the graph to be a downward slope graph.

The fractional conversion which started from 0.02 was increasing while the space velocity was dropping till the fractional conversion increases to 1.00 (X_A = 0.02). So, the effect of the fractional conversion on the space velocity causes a drop of the flowrate, if the fractional conversion continues to increase with respect to time and may cause a problem in the production rate.

However, as fractional conversion increases the space velocity of the reactor decreases to a maximum when fractional conversion X_A = 0.02.

4.2.6Effect of Fractional Conversion on Heat Generated Per Unit Volume of Reactor

From Figure 7, the graph below shows the variation of fractional conversion on heat generated per unit volume of reactor.

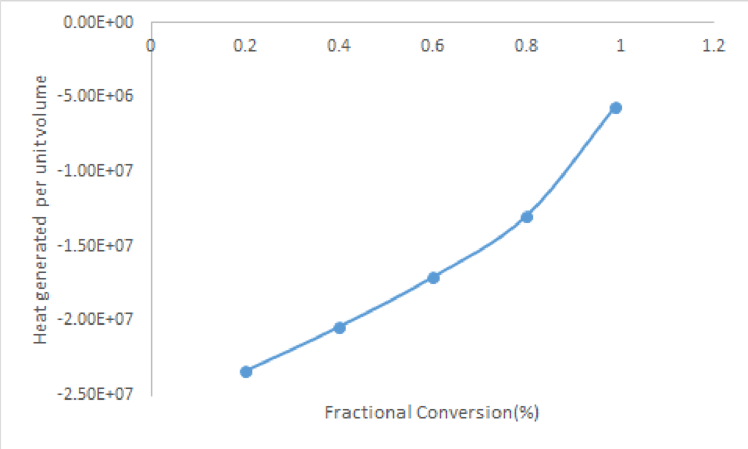


Fig-7: Effect of Fractional Conversion on Heat Generated Per Unit Volume of Reactor

The fractional conversion has an effect on the heat generated per unit volume of the reactor by increasing the heat generated per unit volume of the reactor has fractional conversion increase. The fractional conversion which started from 0.2 causes the heat generated per unit volume of reactor to increase till it attains a maximum heat generated per unit volume of about 173711.6. The increase of the heat generated per unit volume of reactor causes an increase in the fractional conversion which increases the rate of production in the heat generated per unit volume.

However, as the fractional conversion increase, the heat generated per unit volume of the reactor increases, the heat generated per unit volume became maximum as fractional conversion increases to X_A = 0.99. Hence, the cause of increase in the fractional conversion which causes increase in the heat generated per unit volume of reactor makes the graph to be upward slope graph (curve).

4.2.7Effect of Fractional Conversion on Pressure Drop along the Length of Reactor

From Figure 8, the graph below shows the variation of fractional conversion on pressure drop along the length of reactor.

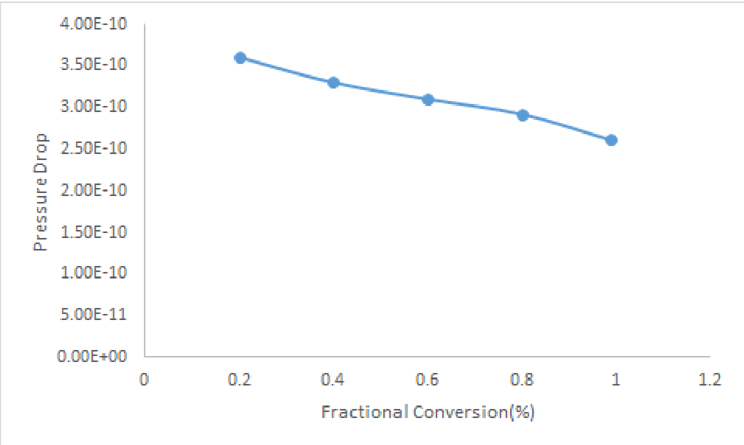


Fig-8: Effect of Fractional Conversion on Pressure Drop along the Length of Reactor

The fractional conversion causes a negative effect on the pressure drop along the length by causing the graph to be a downward slope graph.

The fractional conversion which started from 0.2 was increasing while the pressure drop along the length was dropping till the fractional conversion increases to 0.2 (X_A = 0.2). So, the effect of the fractional conversion on the pressure drop along the length causes a drop of the flow rate, if the fractional conversion continues to increase with respect to time and may cause a problem in the production rate.

However, as fractional conversion increases the pressure drop along the length of the reactor decreases to a maximum when fractional conversion X_A = 0.2.

4.2.8Effect of Net Area on Area of the Column

From Figure 9, the graph below shows the variation of Net area on area of the column.

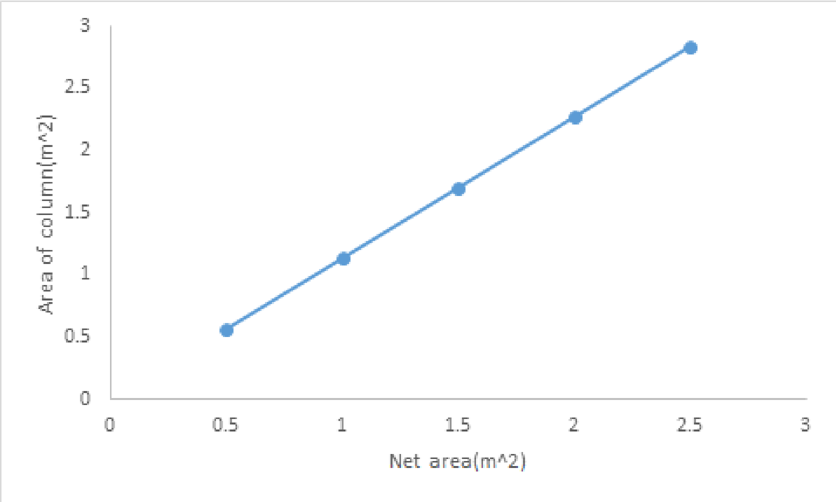


Fig-9: Effect of Net Area on Area of the Column

The net area of the distillation column has an effect on the area of the distillation column by causing the graph to be upward slope graph (positive graph). So, as the net area increases the area of the distillation column also increases the area of the distillation column also increases which then causes an increases in the production at the distillation column. The net area increases from 0.5m^2 to 2.5m^2 while the area of the distillation column increases from 0.57m^2 to 2.84m^2 causing the graph to become a straight line graph slope raising from down to up. However, as net area increases the total area of the distillation column also increases alongside.

4.2.9Effect of Net Area on Diameter of Column

From Figure 10, the graph below shows the variation of Net area on diameter of column.

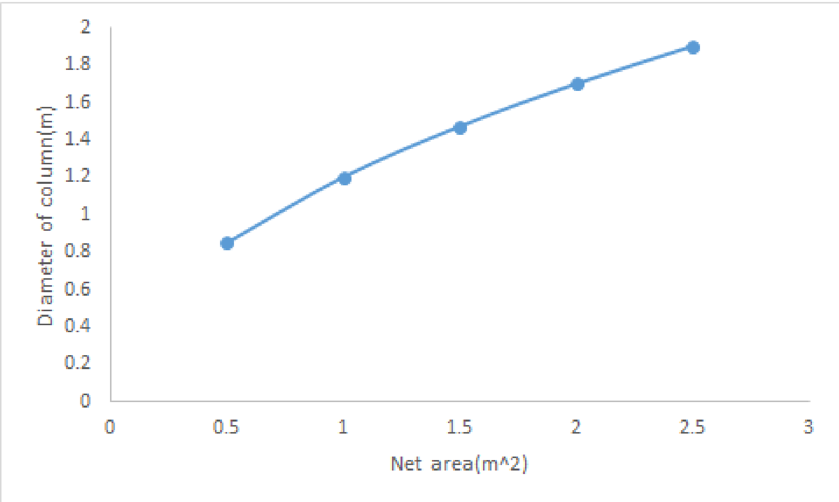


Fig-10: Effect of Net Area on Diameter of Column

The net area of the distillation column has an effect on the diameter of the distillation column by causing the graph to be upward slope graph (positive graph). So, as the net area increases the diameter of the distillation column also increases the area of the distillation column also increases which then causes an increases in the production at the distillation column. The net area increases from 0.5m^2 to 2.5m^2 while the diameter of the distillation column increases from 0.07m^2 to 0.34m^2 causing the graph to become a straight line graph slope raising from down to up. However, as net area increases the diameter of the distillation column also increases alongside.

4.2.10 Effect of Net Area on Down comer Area of the Column

From Figure 11, the graph shows the variation of the net area on down comer area of the column.

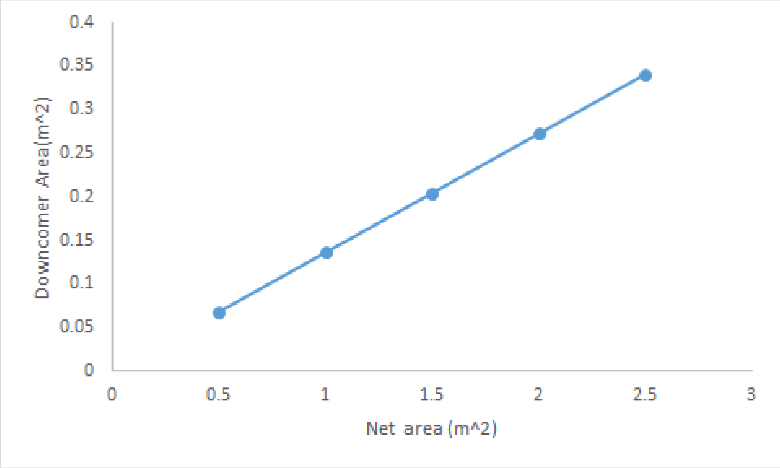


Fig-11: Effect of Net Area of Down comer Area of the Column

The net area of the distillation column has an effect on the down comer area of the distillation column by causing the graph to be upward slope graph (positive graph). So, as the net area increases the down comer area of the distillation column also increases the area of the distillation column also increases which then causes an increases in the production at the distillation column. The net area increases from $0.5m^2$ to $2.5m^2$ while the down comer area of the distillation column increases from 0.85m to 1.90m causing the graph to become a straight line graph slope raising from down to up. However, as net area increases the down comer area of the distillation column also increases alongside.

4.2.11 Effect of Net Area on Weir Length of the Column

From Figure 12, the graph shows the variation of net area on weir length of the column.

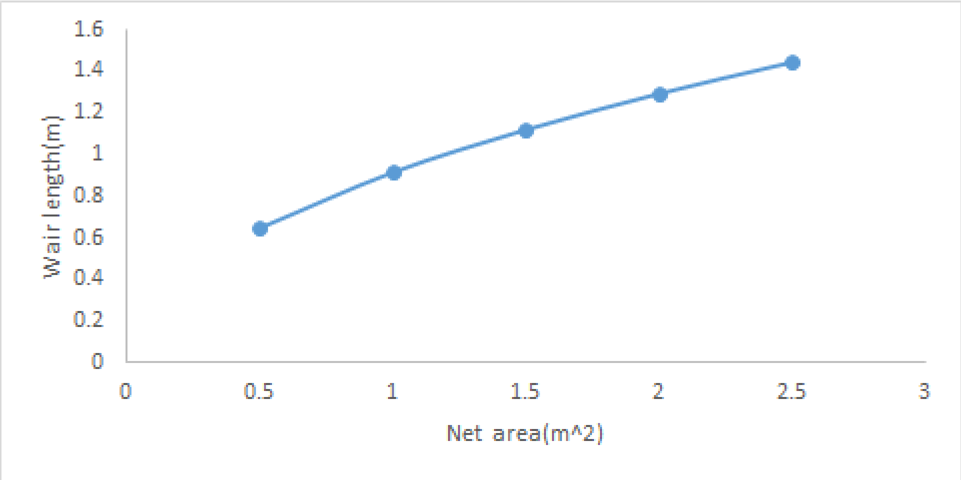


Fig-12: Effect of Net Area of Weir Length of the Column

The net area of the distillation column has an effect on the weir length of the distillation column by causing the graph to be upward slope graph (positive graph). So, as the net area increases the weir length of the distillation column also increases the area of the distillation column also increases which then causes an increases in the production at the distillation column. The net area increases from $0.5m^2$ to $2.5m^2$ while the weir length of the distillation column increases from 0.65m to 1.45m causing the graph to become a straight line graph slope raising from down to up. However, as net area increases the weir length of the distillation column also increases alongside.

4.2.12 Effect of Molar Flow Rate on Area of Packed Bed Column

From Figure 13, the graph shows that as molar flow rate increases then the area of packed bed column increases as well.

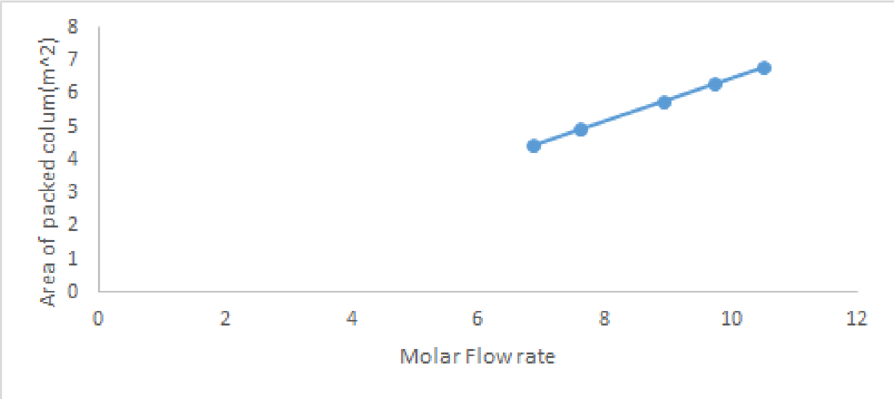


Fig-13: Effect of Molar Flow Rate on Area of Packed Bed Column

The effect of molar flow rate on the area of the packed bed column causes the graph to be an upward slope graph (positive graph). So, as the molar flow rate of the packed bed column increases the area of packed bed column also increases which causes a large increase in the production of 2-ethylhexanol in the packed bed column. The molar flow rate increases from 6.87 to 10.52 while the area of packed bed column increases from 4.44 to 6.80 which causing the graph to become a straight line upward (rising) slope.

However, the increase in area of packed bed column causes an increase in the molar flow rate of the packed bed column for the production of 2-ethylhexanol.

4.2.13 Effect of Molar Flow Rate on Diameter of Packed Bed Column

From Figure 14, the graph below shows that the variation of molar flow rate with diameter of packed bed column.

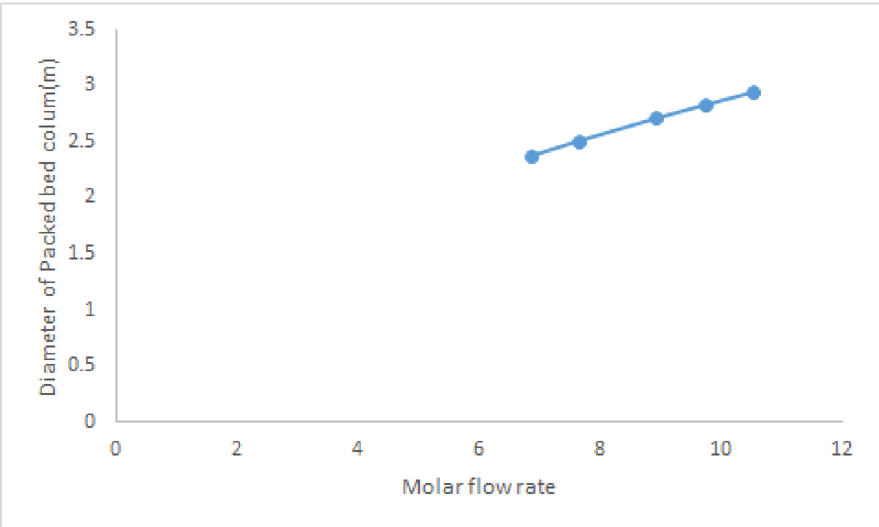


Fig-14: Effect of Molar Flow Rate on Diameter of Packed Bed Column

The effect of molar flow rate on the diameter of the packed bed column causes the graph to be an upward slope graph (positive graph). So, as the molar flow rate of the packed bed column increases the diameter of packed bed column also increases which causes a large increase in the production of 2-ethylhexanol in the packed bed column. The molar flow rate increases from 6.87 to 10.52 while the diameter of packed bed column increases from 2.38 to 2.94 which causing the graph to become a straight line upward (rising) slope.

However, the increase in diameter of packed bed column causes an increase in the molar flow rate of the packed bed column for the production of 2-ethylhexanol.

4.2.14 Effect of Molar Flow Rate on height of Packed Bed Column

From Figure 15, the graph shows the variation of molar flow rate on height of packed bed column.

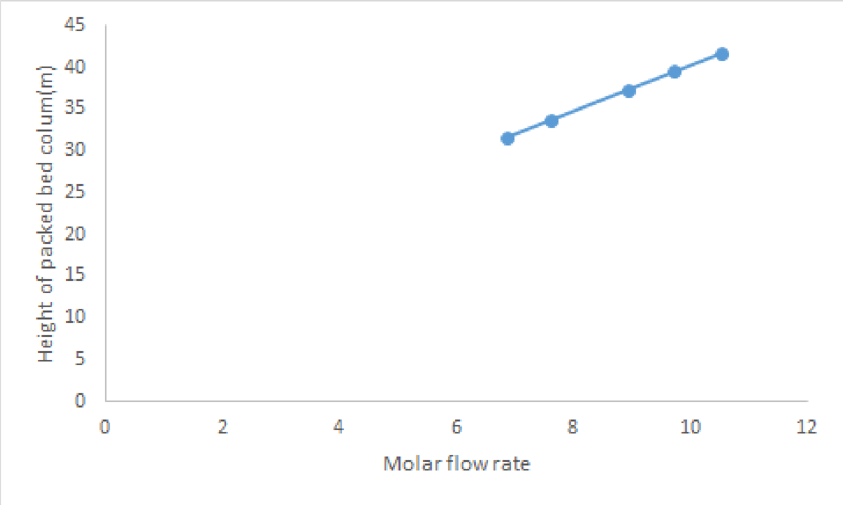


Fig-15: Effect of Molar Flow Rate on Height of Packed Bed Column

The effect of molar flow rate on the height of the packed bed column causes the graph to be an upward slope graph (positive graph). So, as the molar flow rate of the packed bed column increases the height of packed bed column also increases which causes a large increase in the production of 2-ethylhexanol in the packed bed column. The molar flow rate increases from 6.87 to 10.52 while the height of packed bed column increases from 31.66 to 41.65 which causing the graph to become a straight line upward (rising) slope.

However, the increase in height of packed bed column causes an increase in the molar flow rate of the packed bed column for the production of 2-ethylhexanol.

CONCLUSION

The design of distillation column, plug flow reactor and packed column separator for the production of 2-ethylhexanol from propylene and synthesis gas which are the major units in the plant was consider in the work.

The methodology for the design of distillation column, plug flow reactor and packed column separator for the production of 2-ethylhexanol from propylene and synthesis gas was done from the basic principles of material balance (law of conservation of mass). This law of conservation of mass was used to develop the models equations for the distillation column, plug flow reactor and packed column separator for the production of 2-ethylhexanol from propylene and synthesis gas and also the development of the kinetic of the reaction.

The model equations were developing for the plug flow reactor is: The volume of the reactor, length of the reactor, space time, space velocity, heat generated per unit volume and pressure drop along the reactor. The model parameter developed for the distillation column are: rectifying section vapour flow rate, rectifying section liquid flow rate, stripping section vapour flow rate, stripping section liquid flow rate, distillation diameter, height of distillation, down corner area, wet area, weir dimension, hole dimensions and cross-sectional area while the model parameter developed for the separator are: The cross-sectional area, the diameter of the separator, and the height of the separator.

The process diagram for the plant showing the major equipment plug flow reactor, separator and distillation where use to indicate the application of the equipment in the plant and some necessary parameters where also indicated in the schematic diagram. The plant was also sketched with the ASPEN HYSYS, just to show the locations of the equipment design in the work.

Hence, the design parameter gotten from the developed model was simulated and solved with MATLAB and SIMULINK compiler to obtain results which was used to compare with the results of the manual calculations. The results obtain was used to form tables and shows the relationship between different parameters in the distillation column, plug flow reaction and packed column separator for the production of 2-ethylhexanol from propylene and synthesis gas.

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NOMENCLATURE

Abbreviation	**Meaning**
CH_3CHCH_2	Propylene
CO	Carbon-monoxide
H_2	Hydrogen gas
$CH_3CH_2CH_2CHO$	Normal-Butyraldehyde
$CH_3CH_2CH_2C_3H_6CH_2CHO$	Butyraldol
$CH_3CH_2CH_2CHC_3H_5CHO$	Ethylpropyl Acrolein
$CH_3CH_2CH_2CH_2CH_3H_6CHO$	2-Ethylhexanal
$CH_3CH_2CH_2CH_2C_3H_6CH_2OH$	2-Ethylhexanol

SYMBOL	**DESCRIPTION**	**UNIT**
F_A	Molar flow rate of component, A	$mghr^{-1}$
F_{AO}	Initial Molar flow rate of component, A	$mghr^{-1}$
V_r	Volume of Reactor	m^3
X_A	Fractional conversion of component, A	%
D_r	Diameter of Reactor	m
L_r	Length of Reactor	m
S_T	Space Time	S
S_V	Space Velocity	ms^1
ρ	Density of the flowing material	kgm^{-3}
μ	Main fluid viscosity	NSm^{-2}
ΔP	Pressure drop per bar	ms^{-1}
U	Mean superficial velocity	Kpa
V_n	Flow rate of vapour in plate, n	$mghr^{-1}$
L_{n+1}	Flow rate of liquid in plate, n	$mghr^{-1}$
D	Flow rate of density	$mghr^{-1}$
Y_n	Fractional conversion in plate, n	%
X_d	Fractional conversion in distillate	%
V_m	Flow rate of vapour in plate, m	$mghr^{-1}$
L_{m+1}	Flow rate of liquid in plate, m	$mghr^{-1}$
B	Flow rate of bottom product	$mghr^{-1}$
q	Heat required in vaporized	Cm^{-3}
λ	Latent heat of vapourization	
A_C	Column cross-sectional area	m^2
D_C	Column Diameter	m
H_C	Actual column height	m
N_a	Actual number of plate	
H_S	Plate spacing	m
H	Additional height required for the column operation	m
A_d	Down corner area	m^2
A_w	Wet area	m^2
L_w	Weir length	m
A_h	Hole area	m^2
H_d	Hole diameter or size	m
H_P	Hole pitch	m
A_{cp}	Area of packed bed column	m^2
D_{cp}	Diameter of packed bed column	m
H_{og}	Height of packed bed column	m
V_o	Feed volumetric flow rate	m^2s^{-1}
X_f	Mole fraction in the distillate	mol
X_d	Mole fraction the bottom	mol