Department of

Chemical Engineering

Separation Processes

(CHE-421)

Distillation Column Design for Binary mixture of Benzene and Cumene

By

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TABLE OF CONTACTS

1. ABSTRACT…. 3

2. INTRODUCTION TO DISTILLATION….3

2.1. Batch Columns 3

2.2. Continuous Columns 3

3. PROJECT OBJECTIVE…. 4

4. PROBLEM STATEMENT….4

5. PROPERTIES OF CUMENE….. 5

5.1. Gas Phase Thermochemistry Data 5

5.2. Condensed phase thermochemistry data 5

6. PROPERTIES OF BENZENE….. 5

6.1 Gas Phase Thermochemistry Data 5

6.2 Condensed phase thermochemistry data 6

7. VAPOR LIQUID EQUILIBRIUM CALCULATIONS….6

8. COLUMN VARIABLES CALCULATION… 10

8.1. Number of Trays Using Enthalpy Concentration Method 10

8.2. Column Diameter Calculations 17

9. ASPEN HYSYS V11 SIMULATION….20

10. COST OF THE DISTILATION COLUMN… 23

Reference 24

LIST OF FIGURES

Figure 3-1: Schematic of a distillation column 4

Figure 7-1: BPD for Benzene-Cumene System 9

Figure 7-2: BPD for Equilibrium diagram for (A) benzene & (B) Cumene 9

Figure 8.1: Schematic process diagram 10

Figure 8.2: X_F = Feed Composition, X_w= Bottom Composition, X_D= Top Composition. 11

Figure 8.3: Number of stages using equilibrium diagram. 16

Figure 8.4: Souder's-Brown constant K2. 18

Figure 9-1: Feed stream data. 20

Figure 9-2: The flow diagram of the distillation column. 20

Figure 9-3: Temperature variation in distillation column. 22

Figure 9-4: Composition variation in distillation column. 22

Figure 9-5: flow rates of vapor and liquid in distillation column. 22

Figure 9-6: the diameter of column from aspen hysys. 23

LIST OF TABLES

Table 5-1: Gas phase thermochemistry data.[1] 5

Table 5-2: Condensed phase thermochemistry data.[1] 5

Table 6-1: Gas phase thermochemistry data.[2] 5

Table 6-2: Condensed phase thermochemistry data.[2] 6

Table 7-1: Antione equation constants for Benzene-Cumene[3][4][5]. 7

Table 7-2: Vapor liquid equilibrium data for Benzene- cumene mixture 8

Table 8.1: 7-point calculation for enriching section 13

Table 8.2: 7-point calculation for Stripping section 16

Table 9-1: Streams conditions and flow rates. 21

Table 9-2: Condenser and reboiler conditions. 21

Table 10-1: Cost estimation of the distillation tower. 23

1. ABSTRACT

In this study, a general overview of distillation columns will be discussed, and the determination of the equilibrium diagram and data construction first will be performed using Antoine equation of state using constants from chemical engineering literature, followed by the determination of number of stages using enthalpy concentration method for benzene toluene mixture, and third the calculation of the required column diameter under the specified conditions to have no less than 95mol% of the more volatile component which is benzene in this study in the distillate stream. At the end of this report a simulation of the distillation column is performed using ASPEN HYSYS software to simulate the performance of the distillation column for a tray efficiency of 54%, after that an optimization section is added to study the effect of changing the reflux ration on the column performance.

2. INTRODUCTION TO DISTILLATION

A distillation column is an essential device used in the distillation of liquid mixtures to separate the mixture into its component parts, or fractions, based on the differences in volatilities. Fractionating columns are used in small scale laboratory distillations as well as large scale industrial distillations. There are many types of distillation columns, each designed to perform specific types of separations, and each design differs in terms of complexity.

2.1. Batch Columns

In batch operation, the feed to the column is introduced batch-wise. That is, the column is charged with a 'batch' and then the distillation process is carried out. When the desired task is achieved, a next batch of feed is introduced. This type is used in small scale production such as in biological and pharmaceutical separation processes.

2.2. Continuous Columns

In contrast, continuous columns process a continuous feed stream. No interruptions occur unless there is a problem with the column or surrounding process units. They are capable of

handling high throughputs and are the most common of the two types. We shall concentrate only on this class of columns.

The feed to the column can consist either of a binary mixture or a multicomponent mixture. A schematic diagram of a distillation column is shown below in Figure 3.1 with a kettle type reboiler, the enriching section also called the rectifying section represents the section that lays above the feed and the stripping section is the section below the feed. Part of the output overhead product is refluxed back to the column in order to maintain a good vapor-liquid contact in the column as well as to maintain the temperature profile in the column to maintain stage to stage temperatures.

3. PROJECT OBJECTIVE

In this project, a continuous distillation column will be considered in the separation of benzene-cumene mixture using enthalpy concentration method to determine the number of theoretical stages needed. Then the column diameter will be determined as well as an ASPEN HYSYS simulation of the process.

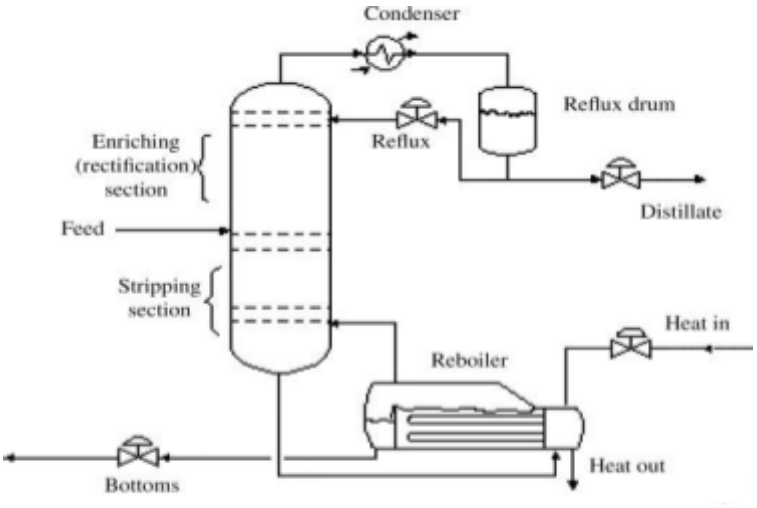


Figure : Schematic of a distillation column

4. PROBLEM STATEMENT

In this report a distillation for a binary mixture of benzene and toluene will be considered to obtain the following results:

- Minimum number of theoretical trays using McCabe-Thiele method.
- Minimum number of theoretical trays using enthalpy concentration method.
- Simulation using ASPEN HYSYS.

The feed stream enters the column at a pressure of 1 atm as saturated vapor at a rate of 100 Kmol/h, the feed is equimolar of benzene and cumene. The preliminary design requirements for the distillate are to contain 95 mol% of Benzene (A) and the bottom waste stream to contain 90 mol% cumene (B).

5. PROPERTIES OF CUMENE

5.1. Gas Phase Thermochemistry Data

In the Table 5-1 the enthalpy and entropy for gas cumene

Table 5-1: Gas phase thermochemistry data.[1]

Quantity	Value	Units
$\Delta_f H°_{gas}$	3.9 ± 1.1	kJ/mol
$S°_{gas}$	386.53	J/mol.K

5.2. Condensed phase thermochemistry data

In the Table 5-2 the enthalpy and entropy for liquid cumene

Table 5-2: Condensed phase thermochemistry data.[1]

Quantity	Value	Units
$\Delta_c H°_{liquid}$	-5218.6	kJ/mol
$S°_{liquid}$	277.57	J/mol.K

6. PROPERTIES OF BENZENE

6.1 Gas Phase Thermochemistry Data

In the Table 6-1 the enthalpy and heat capacity for gas benzene

Table 6-1: Gas phase thermochemistry data.[2]

Quantity	Value	Units
$\Delta_f H°_{gas}$	82.8	kJ/mol
$C_{p,gas}$ (at 273.15 K)	74.55	J/mol.K

6.2 Condensed phase thermochemistry data

In the Table 6-2 the enthalpy and heat capacity for gas benzene

Table 6-2: Condensed phase thermochemistry data.[2]

Quantity	Value	Units
$\Delta_f H°_{liquid}$	46.0	kJ/mol
$S°_{liquid}$	173.26	J/mol.K
$C_{p,liquid}$ (at 300 K)	136.5	J/mol.K

7. VAPOR LIQUID EQUILIBRIUM CALCULATIONS

Vapor Liquid Equilibrium or VLE calculations are an essential part to take into considerations in the analysis and design of distillation columns. Since the process of distillation is based on the deference of the boiling point of the present components VLE data describe the distribution of the chemical species present in the system. Properties such as relative volatility, vapor Pressures, enthalpy for liquid and vapor phases, mole fractions in both liquid and vapor phase, and boiling points are indeed essential in the calculations and analysis of

distillation columns. VLE boiling point diagrams for binary mixtures are based on temperature ranges from the boiling point of the more volatile component up to the boiling point of the less volatile components. VLE boiling point diagrams can be constructed using equations of state such as Antione equation. Antione equation (1) depends on several constant variables for several temperature ranges and are obtained by experiments these variables A, B, and C can be found in the literature.

$$\log_{10}(P^s) = A - \frac{B}{T+C} \quad (1)$$

where P^s is the vapor pressure of the pure component in mmHg and T is the temperature in ˚C. In this report a binary mixture of benzene and cumene is considered and the values of A, B, and C are listed in Table 1 below.

Table 7-1: Antione equation constants for Benzene-Cumene[3][4][5].

Compound	A	B	C	Normal Boiling Point T_b ˚C
Benzene	6.89272	1203.531	219.8	80.1
Cumene	7.10691	1577.97	220.977	151.4

$$P^s_A X_A + P^s_B (1 - X_A) = P_{total} \quad (2)$$

Where P^s_B is the vapor pressure of cumene (B) in mmHg and P_{total} is the total system pressure which is considered as 1 atm or 760 mmHg. Equation (3) shows how the mole fraction of the vapor phase can be obtained.

$$Y_A = \frac{P^S_{A\ X_A}}{P_{total}} \quad (3)$$

Calculation Example

For P_{total} = 101.325 kPa the mole fraction of benzene in the liquid phase at 85.1 ˚C. using equation (1) and Table 1:

$$\log_{10}(P^s_A) = 6.89272 - \frac{1203.531}{90.29+219.8} = 3.011$$

$$P^s_A = 135.52\text{kPa}$$

Similarly:

$$\log_{10}(P^s_B) = 7.1069 - \frac{1577.97}{90.29+220.977} = 2.04$$

$$P^s_B = 14.385\text{kPa}$$

Then equation (2) is used to determine the liquid mole fraction (X_A)

$$P^s_A X_A + P^s_B (1 - X_A) = P_{total}$$

$$(135.52\text{kPa})\, X_A + (14.385\ \text{kPa})\,(1 - X_A) = 101.325\ \text{kPa}$$

Therefore: $X_A = 0.7$.

Equation (3) can be used to determine the mole fraction of the vapor phase as follows:

$$\mathbf{Y_A} = \frac{(135.522kPa)(0.7)}{101.325kPa} = \mathbf{0.96}$$

Now a table can be constructed in a similar manner is this example the data obtained are listed in Table 7.2 below.

Table 7-2: Vapor liquid equilibrium data for Benzene- cumene mixture

T	Vap. kPa	Vap. kPb	Xa	Ya
80.10	100.043	9.692	1.0	1.0
90.29	135.522	14.385	0.7	0.96
100.47	180.072	20.823	0.5	0.9
110.66	235.112	29.466	0.3	0.8
120.84	302.118	40.842	0.2	0.7
131.03	382.609	55.550	0.1	0.5

141.21	478.129	74.260	0.1	0.3
151.40	590.232	97.707	0.0	0.0

When Y_A and X_A are plotted in a single plot against the temperature, the curves can be used to determine the boiling point of the mixture at any desired composition. This boiling point diagram or BPV is shown in Figure 7.1. In Figure 7.2 when the mole fraction of the vapor phase (Y_A) is plotted against the mole fraction of the liquid phase (X_A) a curved line is generated, this curved line is called the 'Equilibrium Line' this line represents the distribution of a substance between the vapor and liquid phase, and it will be used to determine the number of theoretical stages used in the distillation column. This curve is also used to approximate the equilibrium composition of the stages and the optimum feed stage location, the procedure will be discussed in the upcoming sections.

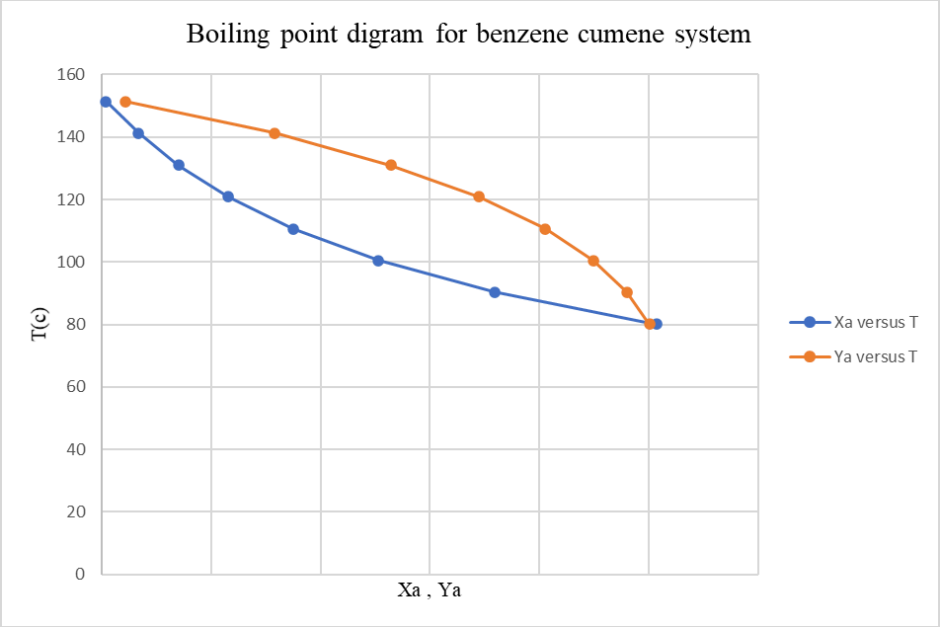


Figure 7-1: BPD for Benzene-Cumene System

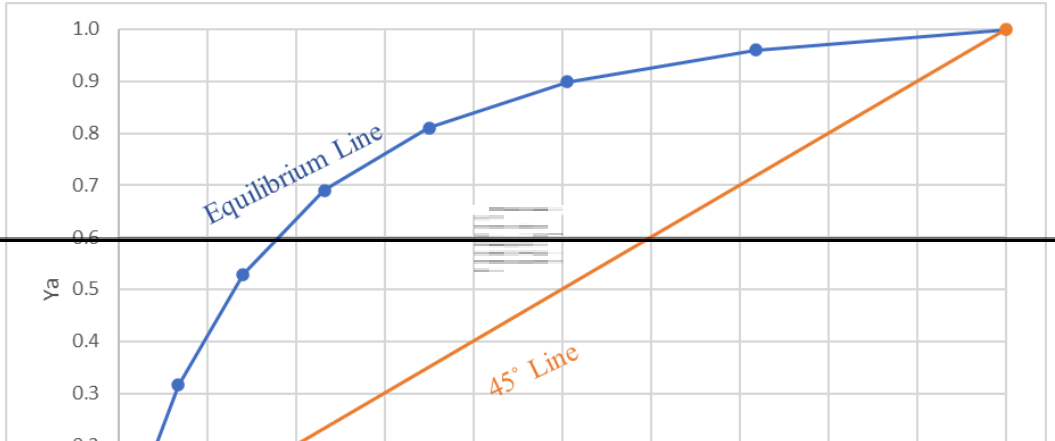
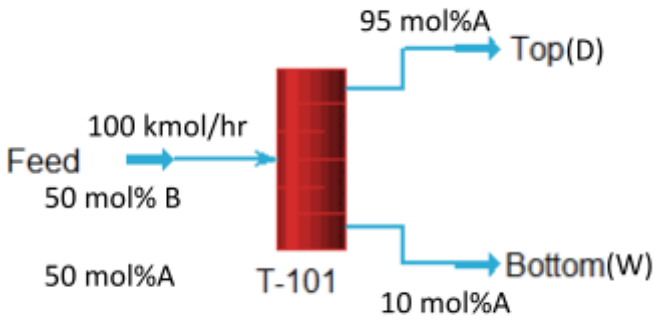


Figure 7-2: BPD for Equilibrium diagram for (A) benzene & (B) Cumene

8. COLUMN VARIABLES CALCULATION

8.1. Number of Trays Using Enthalpy Concentration Method

As discussed in the problem statement the feed conditions and specified purity of the benzene and toluene at the top and bottom respectively are shown in the schematic diagram below:



By applying overall material balance:

$$F = 100 \text{ kmol/h} = D + W$$

$$D = 100 - W \qquad (A)$$

Applying material balance on component A:

$$(0.5)\,(100) = (0.95)\,(D) + (0.1)\,(W) \qquad (B)$$

Solving equation, (A) and (B) yields:

$$W = 52.9 \text{ kmol/hr}$$

$$D = 47.1 \text{ kmol/hr}$$

Now the minimum reflux ratio (R_{min}) needs to be determined, this is done graphically by using Figure 8.2 as shown below:

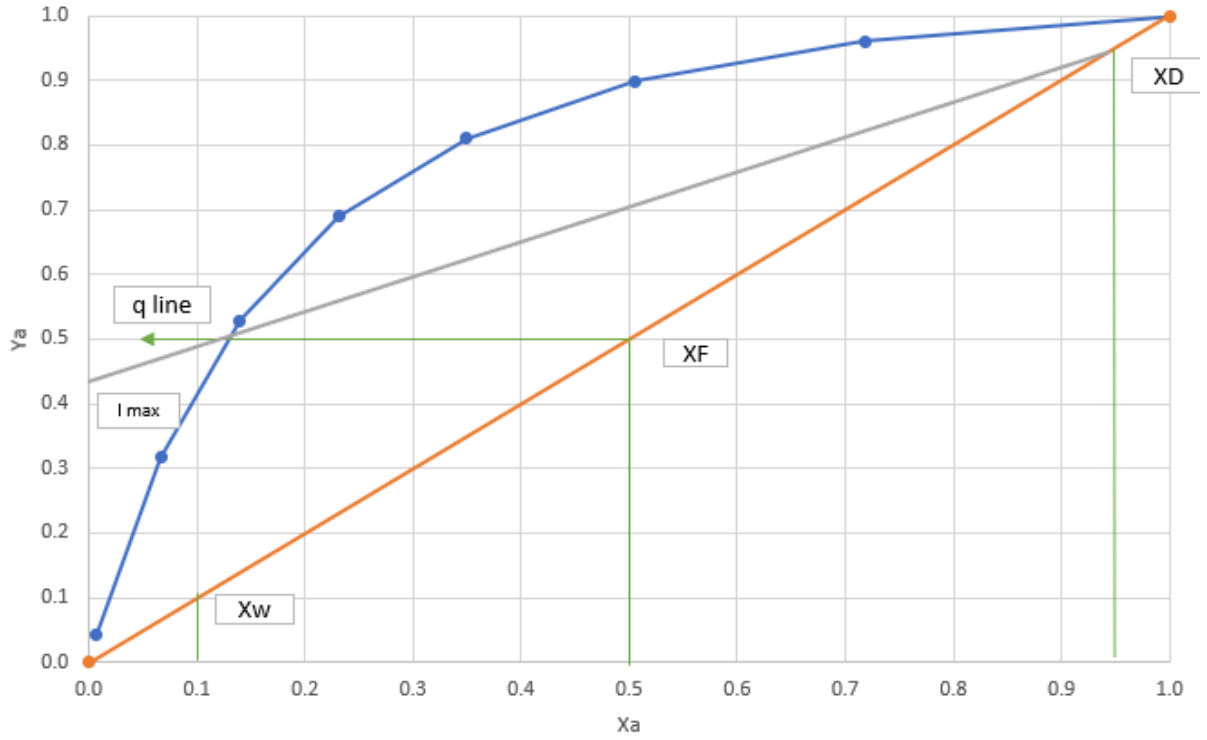


Figure 8.2: X_F = Feed Composition, X_w= Bottom Composition, X_D= Top Composition.

The intercept from Figure 8.2 is I_{max} = 0.43, so the minimum reflux ratio (Rmin) is calculated by Equation (4) which is as follows:

$$I_{max} = \frac{x_D}{R_{min}+1} \qquad (4)$$

$$0.43 = \frac{0.95}{R_{min}+1}$$

$$R_{min} = 1.21$$

The operating reflux ratio is assumed to be 1.5 of the minimum refluxes, therefore:

$$R = 1.5\ R_{min} = (1.5)\ (1.21) = 1.81$$

The Reflux rate = L = R x D = 1.81× 47.1 kmol/hr = 85.251 kmol/hr.

The overhead vapor rate from the column = V_1 = L + D = 85.251 + 47.1 = 132.351 kmol/hr.

The modified latent heat of vaporization of Toluene is calculated be equation (5)

$$ג_B = c_{PB}\left(T_{bB} - T_o\right) + ג_{Bb} - c_{PyB}\left(T_{bB} - T_o\right) \qquad (5)$$

$ג_B = 264.4 * (151.4 - 80.1) + 45100 - 213.2 * (151.4 - 80.1)$ = 48751.27 KJ/Kmol

For enriching section assuming Xn = 0.55 to calculate 0.85 by equation 6:

$$y_{n+1} = \frac{L_n}{V_{n+1}} X_n + \frac{Dx_D}{V_{n+1}} \qquad (6)$$

$$y_{n+1} = \frac{85.25}{132.35}\ 0.55 + \frac{(47.1)(0.95)}{132.35} = 0.692$$

The liquid enthalpy for the top of column in enriching section at X_D = 0.95 at T = 82˚C is by equation 7:

$$hD = x_A\, C_{PA}\left(T - T_o\right) + \left(1 - x_A\right)(c_{PB})\left(T - T_o\right) + \Delta H_{sol} \qquad (7)$$

$hD = 0.95 * 138.2(82 - 80.1) + (1 - 0.95)(264.4)(82 - 80.1) + 0 = 274.57\ KJ/Kmol$

The vapor enthalpy for the top of column in enriching section at Y_1 = 0.95, at T = 91 ˚C is by equation 8:

$$H1 = y_A[ג_A + c_{PyA}\left(T - T_o\right)] + (1 - y_A)[ג_B + c_{PyB}\left(T - T_o\right)] \qquad (8)$$

$H1 = 0.97[30820 + 96.3(91 - 80.1)] + (1 - 0.97)[48751.3 + 213.2(91 - 80.1)]$

= 32445.83 KJ/Kmol

The liquid enthalpy for enriching section at Xn = 0.55, at T = 98 is by equation 7

$$hn = x_A * C_{PA}\left(T - T_o\right) + \left(1 - x_A\right) * c_{PB} * \left(T - T_o\right) + \Delta H_{sol} \qquad (7)$$

$hn = 0.55 * 138.2(98 - 80.1) + (1 - 0.55)(264.4)(98 - 80.1) + 0 = 3490.4\ KJ/Kmol$

The vapor enthalpy for the top of column in enriching section at Y_{n+1}= 0.692, at T = 121 ˚C is by using equation 8:

$$Hn + 1 = y_A[ג_A + c_{PyA}(T - T_o)] + (1 - y_A)[ג_B + c_{PyB}(T - T_o)] \quad (8)$$

$$Hn + 1 = 0.692\,[30820 + 96.3(121 - 80.1)] + (1 - 0.692)[48751.3 + 213.2(121 - 80.1)]$$

= 41746.19 KJ/Kmol

The amount of vapor flow in the enriching section at Xn = 0.55 can be calculated using equation 9 as follows:

$$V_{n+1}H_{n+1} = (V_{n+1} - D)\,h_n + V_1 H_1 + L\,h_D \quad (9)$$

$$V_{n+1}(41746.19) = (V_{n+1} - 47.1)\,(3490.4) + (132.35)\,(32445.83) + (85.25)\,(274.57)$$

$$V_{n+1} = 107.34\ kmol/hr$$

The amount of liquid flow in the enriching section at Xn = 0.55 can be calculated using equation 10 as follows:

$$L_n = V_{n+1} - D \quad (10)$$

$$L_n = 107.34 - 47.1 = 60.24\ \text{kmol/hr}$$

In a similar manner, other iterations can be performed using spreadsheet software as shown in Table 10.1:

Table 8.1: 7-point calculation for enriching section

Enriching section										
Xn	Tn,x (°C)	Tn,y (°C)	yn+1	Vn+1 (kmol/h)	Ln (Kmol/h)	hD (KJ/kmol)	hn (KJ/kmol)	H1 (KJ/kmol)	Hn+1 (KJ/kmol)	qc (KJ/h)
0.55	98	121	0.692	107.34	60.24	274.57	3490.40	32445.83	41746.19	4257899
0.60	96	119	0.725	109.37	62.27		3000.08		40757.71	
0.65	94	116	0.757	111.82	64.72		2534.99		39659.55	
0.70	91	113	0.789	114.02	66.92		1919.09		38583.97	
0.75	89	110	0.821	116.59	69.49		1510.80		37530.99	
0.80	86	105	0.853	119.67	72.57		964.31		36273.72	

0.85	85	98	0.886	124.31	77.21		769.94		34834.75	

Now, calculation for condenser and reboiler duties by equation 11 and 12, respectively:

$$q_c = V_1 H_1 - Lh_D - Dh_D \quad (11)$$

$$qR = Dh_D + Wh_W + q_C - Fh_F \quad (12)$$

The calculation for the condenser duty by equation 11 is as follows:

$$q_c = (132.35)(32445.83) - (82.25)(274.57) - (47.1)(274.57)$$

$$q_c = 4257899\ KJ/h$$

The calculation for the reboiler duty by equation 12 must provides h_W and h_F, so to calculate the h_W for liquid mole fraction in the bottom X_W = 0.1 at T=137 °C and the h_F for liquid mole fraction in the feed X_F = 0.5 at T = 98 °C is by equation 7 as follows:

$$hw = x_A C_{PA}\left(T - T_o\right) + \left(1 - x_A\right)(c_{PB})\left(T - T_o\right) + \Delta H_{sol} \quad (7)$$

$$hF = x_A C_{PA}\left(T - T_o\right) + \left(1 - x_A\right)(c_{PB})\left(T - T_o\right) + \Delta H_{sol} \quad (7)$$

$$hw = 0.1 * 138.2(137 - 80.1) + (1 - 0.1)(264.4)(137 - 80.1) + 0 = 14326.79\ KJ/Kmol$$

$$hF = 0.5 * 138.2(98 - 80.1) + (1 - 0.5)(264.4)(98 - 80.1) + 0 = 3603.36\ KJ/Kmol$$

so the reboiler duty is as follows:

$$qR = (47.1)(274.57) + (52.9)(14326.79) + (4257899) - (100)(3603.36)$$

$$qR = 4668383\ KJ/h$$

Now the calculation for the stripping section, started by assuming points for y_{m+1} and calculating x_m among the down section of the tower by equation 13. The first iteration is y_{m+1} = 0.25 at T = 105 °C

$$y_{m+1} = \frac{L_m}{V_{m+1}} * x_m - \frac{W * x_W}{V_{m+1}} \quad (13)$$

To calculate L_m and V_m for first iteration is done by equation 14 and 15 as follows:

$$L_m = L + qF \qquad (14)$$

$$V_m = V1 - (1-q)\,F \qquad (15)$$

$L_m = 85.25 + (0)(100) = 85.25$ kmol/h

$V_m = 132.35 - (1-0)\,(100) = 32.35$ kmol/h

So,

$$0.25 = \frac{85.25}{32.35} * x_m - \frac{(52.9)(0.1)}{32.35}$$

$$x_m = 0.4$$

Now to calculate the amount of vapor in stripping section is by equation 16

$$V_{m+1} H_{m+1} = \left(V_{m+1} + W\right)h_m + q_R - Wh_W \qquad (16)$$

To calculate the amount of vapor in stripping section it must provide calculations for the vapor and liquid enthalpies H_{m+1} and h_m and this is done by equation 8 and 7 respectively.

$$Hm + 1 = y_A[\lambda_A + c_{PyA}\left(T - T_o\right)] + (1 - y_A)[\lambda_B + c_{PyB}\left(T - T_o\right)] \qquad (8)$$

$$hm = x_A\, C_{PA}\left(T - T_o\right) + \left(1 - x_A\right)(c_{PB})\left(T - T_o\right) + \Delta H_{sol} \qquad (7)$$

for the vapor enthalpy it calculated at y_{m+1} = 0.25 and at T= 144 °C.

$$Hm + 1 = 0.25\,[30820 + 96.3(144 - 80.1)] + (1 - 0.25)[48751.273 + 213.2(144 - 80.1)]$$

= 56024.46 KJ/Kmol

For the liquid enthalpy it calculated at x_m = 0.214 and at T= 104 °C.

$$hm = (0.214)(138.2)(104 - 80.1) + (1 - 0.214)(264.4)(104 - 80.1) + 0 = 5674.36\ KJ/Kmol$$

back to equation 15 to calculate the amount of vapor:

$$V_{m+1}(56024.46) = \left(V_{m+1} + 52.9\right)(5674.36) + (4264998) - (52.9)\,(6521.34)$$

V_{m+1} [redacted] kmol/h

To calculate the liquid in the stripping section is done by equation 17:

$$L_{m+1} = V_{m+1} + W \qquad (17)$$

$$L_{m+1} = 95.11 + 52.9$$

$$L_{m+1} = 148.01 \text{ kmol/h}$$

In a similar manner, other iterations can be performed using spreadsheet software as shown in Table 8.2:

Table 8.2: 7-point calculation for Stripping section

Stripping section								
ym+1	Tm,y (°C)	xm+1	Tm,x (°C)	Vm+1 (Kmol/h)	Lm+1 (Kmol/h)	Hm+1 (KJ/kmol)	hm+1 (KJ/kmol)	qr (KJ/h)
0.25	144	0.16	119	94.90	147.80	56024.46	9515.13	4668383
0.3	142	0.18	115	94.85	147.75	54398.14	8453.14	
0.35	140	0.19	110	94.02	146.92	52795.2	7170.48	
0.4	137	0.21	107	95.12	148.02	51049.2	6386.62	
0.45	135	0.23	104	95.89	148.79	49498.87	5617.12	
0.5	132	0.25	100	96.22	149.12	47817.16	4629.36	
0.55	130	0.27	98	97.84	150.74	46319.43	4121.24	
0.6	126	0.29	95	99.36	152.26	44558.96	3394.85	

As shown in Figure 8.3 by plotting the mole fractions of the liquid and vapor in the enriching and stripping sections along with VLE data shown in Figure 4.2 gives the operating line of the process, stepping down from the top at $X_D = 0.95$ and $Y_1 = 0.97$ to the bottom at $X_w = 0.1$ and $Y_{n+1} = 0.4$ gives a total number of trays = N = 3.5 = 4 theoretical stages including reboiler.

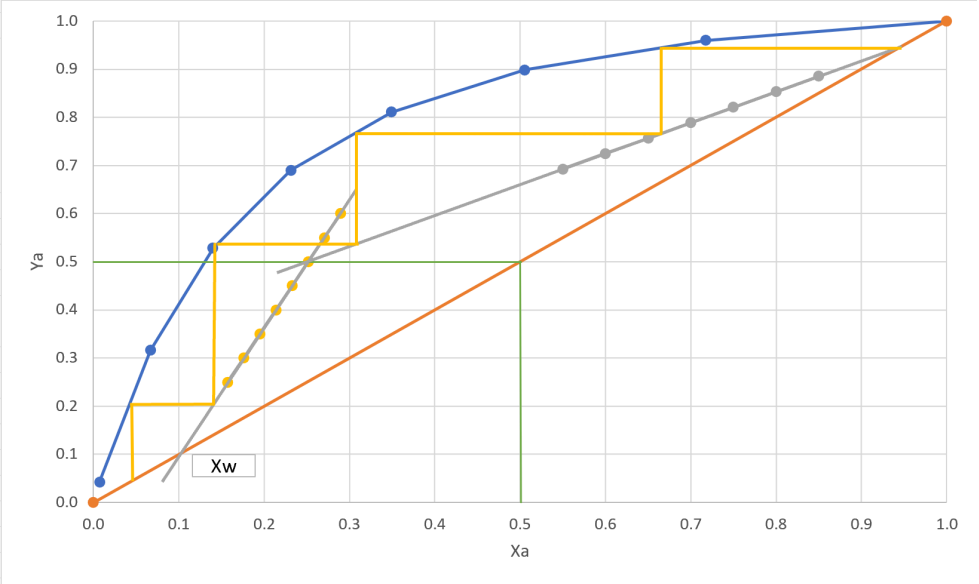


Figure STYLEREF 1 \s 8. SEQ Figure * ARABIC \s 1 3: Number of stages using equilibrium diagram.

8.2. Column Diameter Calculations

Now is the calculation for diameter of the column will be performed. Assuming a plate spacing of 24 inch and a surface tension of 20 dyne/cm. The amounts of liquid and vapor that will be entering the column are as follows:

L = 85.25 kmol/h

V = 104.51 kmol/h

The mole fraction of vapor and liquid respectively:

Y_A =0.4, Y_B=0.6

$$X_A = 0.95\,,\ X_B = 0.05$$

The vapor average molecular weight should be calculating by using equation 18 by taking the molecular weight for each substance from appendix:

$$M_{W,V\ Avg} = y_A M_{WA} + y_B M_{WB} \qquad (18)$$

$M_{W,V\ Avg}$ = (0.4) (78.11) + (0.6) (120.2) = 103.4 kg/kmol

Now to calculate the vapor density for the two substances is by assuming ideal gas system with the feed condition which is at P = 101300 Pa and at T = 80.1 °C. This is done by equation 19

$$p_v = \frac{M_{W,V\,Avg} P}{RT} \qquad (19)$$

$$p_v = \frac{(103.4)(101300)}{8314(80.1+273)} = 3.57\ (kg/m^3)$$

Get average molecular weight as liquid using the liquid mole fraction from equation 17 :

$$M_{W,L\,Avg} = x_A M_{WA} + x_B M_{WB}.$$

$$M_{W,L\,Avg} = 0.95 * 78.11 + 0.05 * 120.2 = 80.21 \text{(kg/kmol)}$$

To calculate the density of liquid, the mass fraction must be obtained as follows:

$$m_A = \left(L\, x_A\right) M_{WA} = (85.25\ )(0.95)(78.11) = 6325.93\ kg/h$$

$$m_B = \left(L\ x_B\right)(M_{WB}) = (104.51)(0.05)(120.2) = 628.11\ kg/h$$

$$m_{tot} = m_A + m_B = 6325.93 + 628.11 = 6954.04 kg/h$$

$$x_A \text{ wt\%} = \frac{m_A}{m_{tot}} = \frac{6325.93}{6954.04} = 0.91$$

$$x_B \text{ wt\%} = 1 - x_A \text{ wt\%} = 1 - 0.91 = 0.09$$

Therefore:

$$p_L = x_A wt\,\% * p_A + x_B wt\,\% * p_B = 0.91 * 876 + 0.09 * 862 = 874.74 kg/m^3$$

Using Figure 10.4, the x-axis value must be determined to find the value of the allowable vapor velocity in the column:

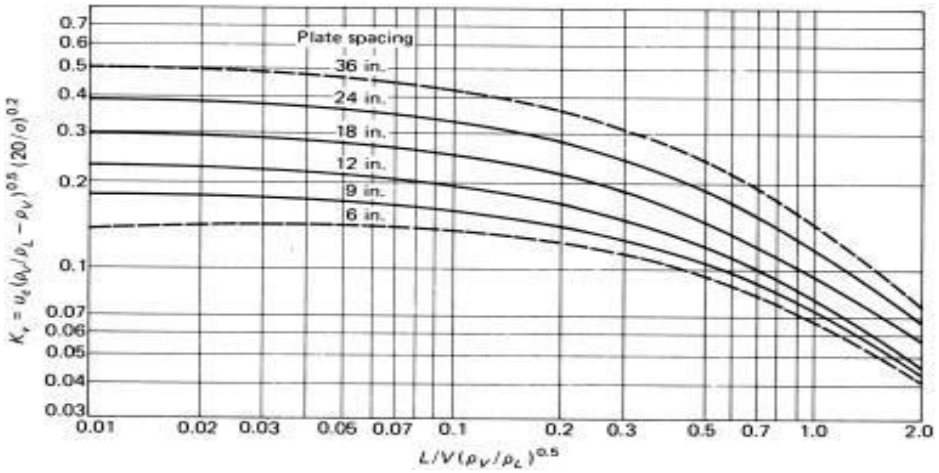
$$V = M_{W,v\,Avg}\, V = (103.4)(104.51) = 10806.334 \text{kg/h})$$

$$L = M_{W,L\,Avg} \quad L = (80.21)(85.21) = 6834.69 \text{ (kg/h)}$$

$$x - axis = \frac{L}{V}\left(\frac{p_v}{p_L}\right)^{0.5} = \frac{10806.33}{6834.69}\left(\frac{3.57}{874.74}\right)^{0.5} = 0.015$$

For 18 in plate spacing get the $K_v(\frac{ft}{s})$:

Figure STYLEREF 1 \s 8. SEQ Figure * ARABIC \s 1 4:
Souder's-Brown constant K2.



The value obtained for the allowable vapor velocity is:

$$K_v = 0.3\left(\frac{ft}{s}\right)$$

σ =20(dyne/cm)

$$v_{max} = K_v * (\frac{o}{20})^{0.2} * \sqrt{\frac{p_L - p_V}{p_V}} = 0.3 * (\frac{20}{20})^{0.2}\sqrt{\frac{874.74-3.57}{3.57}} = 4.69\left(\frac{ft}{s}\right)$$

$$v_{max} = 1.43\ (\frac{m}{s})$$

The correction factors for the design velocity is to multiply by 0.95 to account for foaming, 0.91 to account for the area of the column excluding the downcomer, 0.8 to account for flooding, hence.

v_{Design} = (1.43) (0.91) (0.95) (0.8)=0.99 (m/s)

$$Q = \frac{V}{p_v} = \frac{\left(\frac{10806.334}{3600}\right)}{3.57} = 0.84 m^3/s$$

$$A = \frac{Q}{v_{Design}} = \left(\frac{0.84}{0.99}\right) = 0.85 m^2$$

The column diameter is therefore:

$$D = \sqrt{\frac{4*A}{\pi}} = \sqrt{\frac{4*0.85}{3.14}} = 1.1\, m$$

This column dimeter agrees closely to the diameter obtained by the simulator of 1.5 m in the

next section.

9. ASPEN HYSYS V11 SIMULATION

The simulation is conduct based on the feed data which are shown in Figure 9.1. First a shortcut column method was used to determine the minimum number of stages for a saturated vapor feed, the light key in bottoms is benzene with 10 mol% and the heavy key in distillate is cumene with 5 mol%. The minimum number of trays obtained was 3. By assuming a tray efficiency of 50% of that in the ideal conditions, the actual number of trays is 6. Also, kettle reboiler with a total reflux column will be used in this simulation. The process flow diagram is shown in Figure 9.2.

Stream Name	F.
Vapour / Phase Fraction	1.0000
Temperature [C]	132.6
Pressure [kPa]	101.3
Molar Flow [kgmole/h]	100.0
Mass Flow [kg/h]	9915
Std Ideal Liq Vol Flow [m3/h]	11.38
Molar Enthalpy [kJ/kgmole]	5.813e+004

Figure 9-1: Feed stream data.

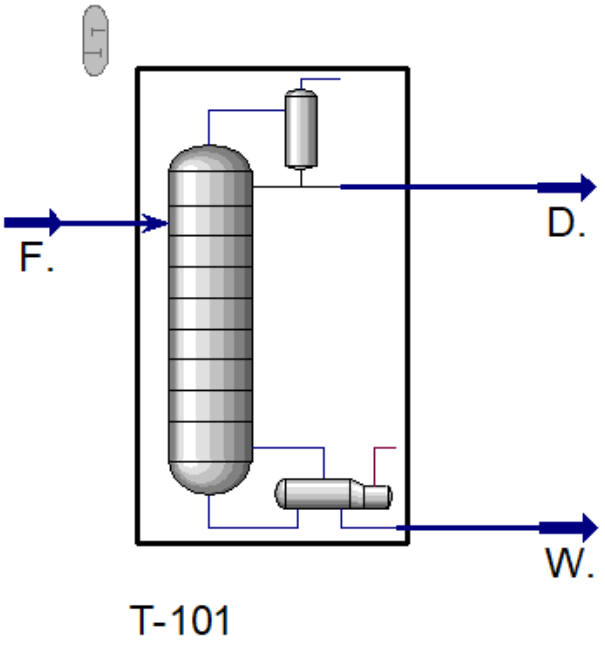


Figure 9-2: The flow diagram of the distillation column.

The data obtained from the simulator are for the composition of benzene at the distillate (D) of X_D equal 92.57 mol% and at the bottom of X_w equal 12.15 mol%. Streams conditions and flow rates are summarized in Table 9.1 below. The duties and data of the condenser and reboiler obtained from the simulator are shown in Table 9.2, the temperature of the condenser can be obtained by using cooling water to condense the outlet vapor and using low pressure steam in reboiler.

Table 9-1: Streams conditions and flow rates.

Name	Feed	To condenser	Reflux	Distillate	To boiler	Boil up	Bottom
Vapor	1	1	0	0	0	1	0
Temperature [C°]	132.6	86.39	82.46	82.46	130.7	133.8	133.8
Pressure [kPa]	101.3	101.3	101.3	101.3	101.3	101.3	101.3
Molar flow rate [kmol/h]	100	131.1	84	47.06	65.10	12.16	52.94
Molar Enthalpy [kJ/kmol]	58129	82842	51322	51322	-678	56733	-5330

Table 9-2: Condenser and reboiler conditions.

Condenser

Type	Total
Temperature	82.46 C
Pressure	101.3 kPa
Duty	4.131e+006 kJ/h

Reboiler

Type	Regular
Temperature	133.8 C
Pressure	101.3 kPa
Duty	4.516e+005 kJ/h

In the case study the pressure is held constant at 1 atm. So, the pressure doesn't change from one tray to another tray. However, the temperature varies from on tray to another, the variation is shown in Figure 9.3. Similarly, the composition also varies along with tray position this is shown in Figure 9.4 where the mole fraction of benzene reaches the set value of X_D equal 92.57 mol% at the condenser stage 0. The flow rates of vapor and liquid in the distillation column at every stage are shown in Figure 9.5. Further optimization of the column will be discussed in the following section to determine the optimum conditions of the column.

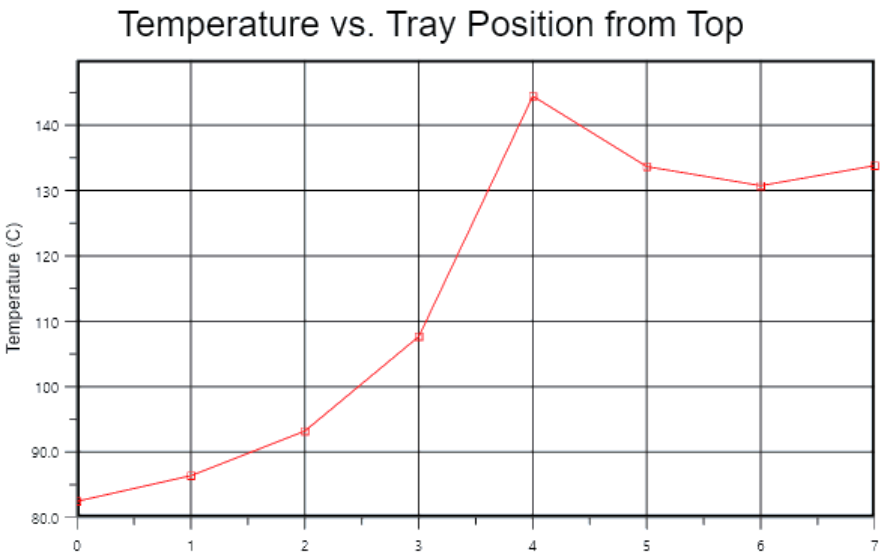


Figure 9-3: Temperature variation in distillation column.

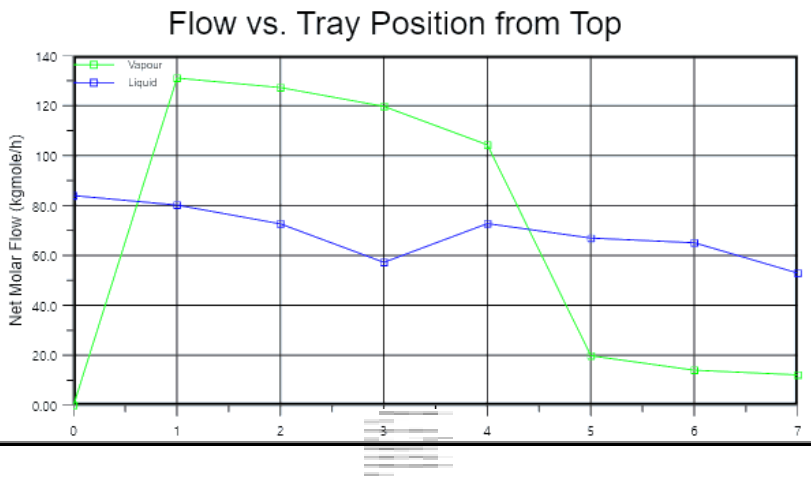


Figure 9-4: Composition variation in distillation column.

Figure 9-5: flow rates of vapor and liquid in distillation column.

The diameter from aspen hysys is 1.5 as show in Figure 9.6.

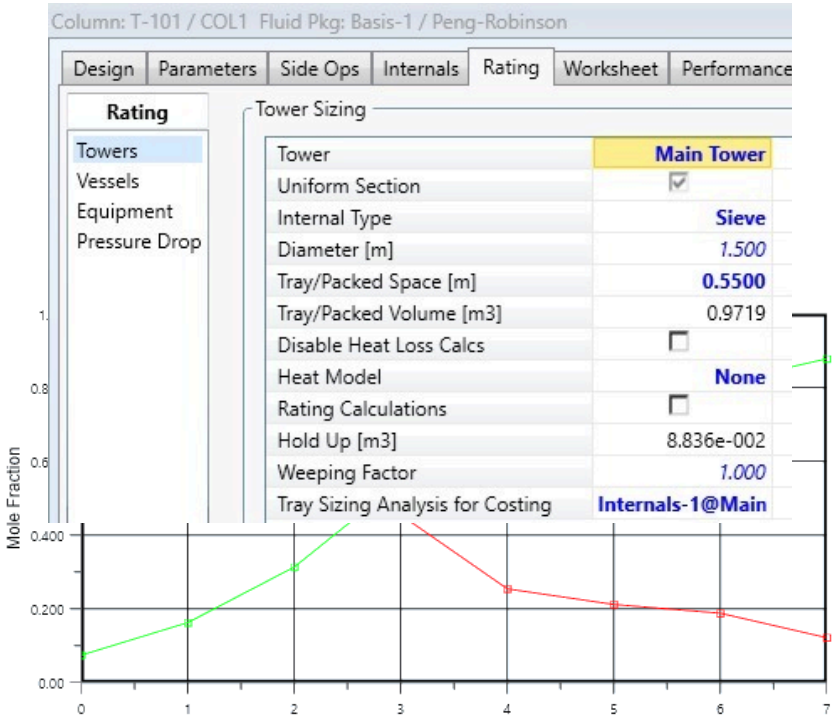


Figure 9-6: the diameter of column from aspen hysys.

10. COST OF THE DISTILATION COLUMN

The total capital cost of the distillation column is 2.59M $. The cost is estimated by Aspen Hysys. The detail of the cost such as utilities and equipment costs are shown in Table 12.1.

Table 10-1: Cost estimation of the distillation tower.

Summary					
Total Capital Cost [USD]					**$2,592,560**
Total Operating Cost [USD/Year]					$1,011,450
Total Utilities Cost [USD/Year]					$ 80,128
Equipment Cost [USD]					$ 100,900
Total Installed Cost [USD]					$ 517,600
Utilities					
Name	**Fluid**	**Rate**	**Rate Units**	**Cost per Hou**	**Cost Units**
Electricity		56.05	KW	$ 4.34	USD/H
Cooling Water	Water	3916468	BTU/H	$ 0.88	USD/H
Steam @100PSI	Steam	0.48152	KLB/H	$ 3.92	USD/H
Equipment					
Name		**Equipment Cost [USD]**		**Installed Cost [USD]**	

Reference

[1] NIST Chemistry Webbook, SDR 69, 2021 by the U.S. Secretary of Commerce on behalf.

< https://webbook.nist.gov/cgi/cbook.cgi?ID=C98828&Mask=3EFF >.2021/11/26, at 6:20 am.

[2] NIST Chemistry Webbook, SDR 69, 2021 by the U.S. Secretary of Commerce on behalf.

<https://webbook.nist.gov/cgi/cbook.cgi?ID=C71432&Mask=2#Thermo-Condensed>
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[5] Principles And Modern Applications Of Mass Transfer Operations, 4th edition 2009, John Wiley & Sons.