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CASE STUDY ON MULTICOMPONENT DISTILLATION AND DISTILLATION COLUMN SEQUENCING

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ABSTRACT

The objective of this work is to design a multi-component distillation column for the given organic mixture, sequencing of a multi-component distillation column to choose the best sequence. Fractionation of multi-component mixtures into top and side stream products depends on the relative volatility of the organic mixture under consideration. As the mixture consists of more than one component with specific true boiling point (TBP), its relative volatility can be calculated using Antoine's equation. In this method the component with the lowest relative volatility at the top above the feed tray was designated as a light key component (LK) and the highest volatility at the bottom, below the feed plate are designated as the heavy key component (HK). Based on these data, the column is designed. Short cut methods involving Fenske's equation, Underwood equation and Gilliland equations, popularly known as the FUG method are employed for the calculations.

A simple heuristic method for the systematic synthesis of initial sequences for Multi-component separations is employed here to determine the best sequence. Therefore the sequence with the least vapour load in turn results in low energy demand, thereby forming the best sequence for the designing of a distillation column for a given organic mixture keeping in mind the economic conditions.

KEYWORDS: Multi component distillation, light key component (LK), heavy key component (HK), Fenske's equation, Underwood equation and Gilliland equation.

INTRODUCTION

Distillation:
Distillation is a separation process that takes advantage of differences in boiling points in a number of vaporization and condensation steps [1]. Distillation column is defined as a device used to separate components of a mixture using the thermodynamic properties of the components [2]. A schematic diagram of a distillation unit with a single feed and two product streams is shown in Figure 1.1.
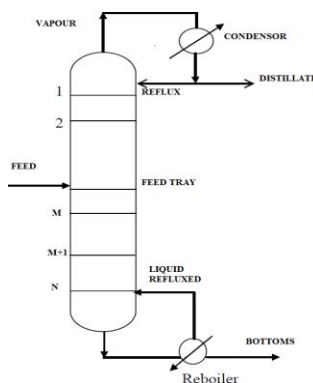

Figure 1.1: Distillation Column.

The column is adiabatic and the initial mixture to be processed, known as the feed, is introduced in the middle of the column to a tray known as the feed tray. The feed tray divides the column into a top (absorption/enriching/ rectification) section and a bottom (stripping/ exhausting) section. Heat is added to the bottom of the column as reboiler heat, and removed at the top as the heat load of the condenser. Essentially, components with lower boiling points will tend toward the top of the column as vapour and the components with higher boiling points will gravitate toward the bottom as liquid.

Inside the column, liquids and vapours are always at their bubble and dew points respectively so that the highest temperatures are at the bottom, the lowest at the top. The reboiler can be considered as a theoretical stage or tray. The entropy and molar flow between the liquid and vapour phases are complex phenomena. Convection, conduction and heat of vaporization take place as the fluids flow through a stage, exchanging heat and mass.

Multicomponent Distillation:

The multi-component separations are carried out by using the binary type of distillation columns, reboilers, condensers, heat exchangers and so on. In multi-component systems, the same degree of freedom (the number of values in the final calculation that are independent or free to vary) is not achieved because of the presence of other components. Neither the distillate nor the bottoms composition is completely specified. The components that have their distillate and bottoms fractional recoveries specified are called key components. The most volatile of the keys is called the light key (LK) and the least volatile is called the heavy key (HK). The other components are called non-keys (NK). Light non-key (LNK) is referred when non-key is more volatile than the light key whereas heavy non-key (HNK) is less volatile than the heavy key. Proper selection of key components is important if a multi-component separation is adequately specified. These involve generally an estimation of the minimum number of trays, the estimation of minimum reflux rate and number of stages at finite reflux for simple fractionators. Although rigorous computer methods are available to solve multi-component separation problems, approximate methods are used in practice.

Multi-component distillation calculations are classified as design or rating methods [3]. In past, the number of stages has to be determined given the recovery of key components while in the latter the composition of products has to be found given the number of stages in the enriching and stripping sections of the distillation column. A widely used approximate method is commonly used to find out the number of stages required is the Fenske-Underwood-Gilliland method (FUG)..

Minimum Number Of Trays (Fenske Equation):

Fenske (1931)[3] was the first to derive an Equation to calculate minimum number of trays for multi-component distillation at total reflux. The derivation was based on the assumptions that the stages are equilibrium stages. Consider a multi-component distillation column operating at total reflux as shown in Figure 1.2.
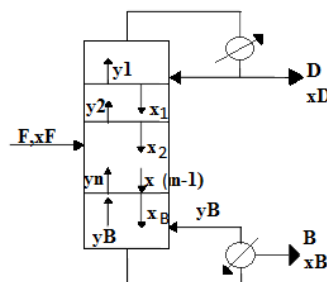

Figure 1.2: Multi-component column at minimum trays.

[4]Equilibrium relation for the light key component on the top tray is

$$y_1 = K_1 x_1 \qquad\qquad (1.3.1)$$

For total condenser, $y_1 = x_D$ then

$$x_D = K_1 x_1 \qquad\qquad (1.3.2)$$

An overall material balance below the top tray and around the top of the column:

$$V_2 = L_1 + D \qquad\qquad (1.3.3)$$

Under total reflux condition, $D = 0$, thus, $V_2 = L_1$. The component material balance for the light key component around the first plate and the top of the column i.

$$V_2 y_2 = L_1 x_1 + D x_D \qquad\qquad (1.3.4)$$

Then under the conditions of the minimum trays, the Equation yields $y_2 = x_1$.

The equilibrium relation for plate 2 is

$$y_2 \; \square \; K_2 x_2 \qquad x_1 \; \square \; K_2 x_2 \qquad x_D \; \square \; K_1 K_2 x_2 \qquad\qquad \ldots(1.3.5, 1.3.6, 1.3.7)$$

Continuing this calculation for entire column, it can be written as:

$$x_D \; \square \; K_1 K_2 \ldots\ldots\ldots K_n K_B x_B \qquad\qquad (1.3.8)$$

In the same fashion, for the heavy key component, it can be written as:

$$x'_D \square\square \; K_1' K_2' \ldots\ldots\ldots K_n' K_B' x'_B \qquad\qquad (1.3.9)$$

We have,

$$\frac{x_D}{x'_D} = \frac{K_1 K_2 \ldots\ldots\ldots K_n K_B x_B}{K_1' K_2' \ldots\ldots\ldots K_n' K_B' x'_B} \qquad\qquad (1.3.10)$$

The ratio of the K values is equal to the relative volatility

$$\frac{x_D}{x'_D} = \alpha_D \alpha_B \qquad\qquad (1.3.11)$$

The above equation can be written even in terms of the vapour composition y. Then on assuming a total condenser and the relative volatility being constant up the column for two components i and j, we get

$$\frac{x_{i,D}}{x_{j,D}} = \alpha_{i,j}{}^{N_{min}} \frac{x_{i,B}}{x_{j,B}} \qquad\qquad (1.3.12)$$

The above equation predicts the number of theoretical stages at total reflux and is known as Fenske Equation[3]. Where **i** is the Light key component and **j** is the heavy key component, and taking their recoveries in distillate and bottom into consideration we get N_{min} with reference to the heavy key component[5 (eq. 9.39)]

N_{min} can also be calculated using the following equation.

$$N_{min} = \frac{\log\left[\frac{r_{L,D}}{1-r_{L,D}} \cdot \frac{r_{H,B}}{1-r_{H,B}}\right]}{\log \alpha_{LH}} \qquad\qquad (1.3.13)$$

Where,
$r_{L,D}$ = recovery of light key component in the distillate,
$r_{H,B}$ = recovery of heavy key component in the bottom ,
$\alpha_{L,H}$ = relative volatility between light and heavy key component

Minimum Reflux Ratio: Underwood Equations

For multi-component systems, if one or more of the components appear in only one of the products, there occurs a separate pinch points in both the stripping and rectifying sections. In this case, Underwood developed an alternative analysis to find the minimum reflux ratio[6]. The minimum reflux ratio is determined by Underwood equations.

Equation 1:

$$\sum_{i=1}^{NC} \frac{\alpha_{ij*} \, x_{i,F}}{\alpha_{ij} - \theta} = \quad 1-q \qquad\qquad (1.4.1)$$

Taking q-value equal to one as the feed is saturated liquid.

Equation 2:

$$\sum_{i=1}^{NC} \alpha_{ij} * \frac{x_{id}}{\alpha_{ij} - \theta} = R_{min} + 1 \qquad\qquad (1.4.2)$$

The flow factor and the tray space is calculated and the column is operated at 85% of the flooding capacity, the number of theoretical trays is then calculated by Gilliland equation [5],

$$\frac{(N - N_{min})}{N + 1} = 1 - e^{\left[\left(\frac{1+\frac{54.4(R-R_{min})}{(R+1)}}{11+\frac{117.2(R-R_{min})}{(R+1)}}\right)\left(\frac{\frac{(R-R_{min})}{(R+1)}-1}{[\frac{(R-R_{min})}{(R+1)}]^{0.5}}\right)\right]}$$

$$(1.4.3)$$

The overall efficiency is calculated by O'Connell equation [7], and hence the number of actual stages and the column height. The column down-comer, net, and active areas are specified as well as the diameter of the column at 85% of the flooding velocity

Distillation Column Secqueing:

Multicomponent separation systems are found in widespread use in the chemical and petroleum industries. An important process design problem in multi component separations is the separation sequencing, which is concerned with the selection of the optimal method and sequence for the separation. Hendry and Hughes [9] introduced the separation task concept, where the distillation network is decomposed into the individual separation tasks, which are evaluated using the ideal thermodynamic based Underwood-Fenske-Gilliland method.

The major problem with column sequencing is the large number of possible sequences, which grows exponential by the number of products. The number of possible sequences for a desired number of products is given by the formula [10]

$$N_s = \frac{(2(P-1))!}{P!(P-1)!} \qquad\qquad (1.5.1)$$

This contribution presents a stepwise procedure to identify the optimal sequence. This problem is often solved by first arranging the components in the mixture to be separated in some ranked lists of appropriate physical and/or chemical properties such as relative volatility.

The sequence shown in the Figure below is known as the direct sequence in which the lightest component is taken overhead in each column. The indirect sequence, as shown in Figure below, it takes the heaviest component as bottom product in each column.
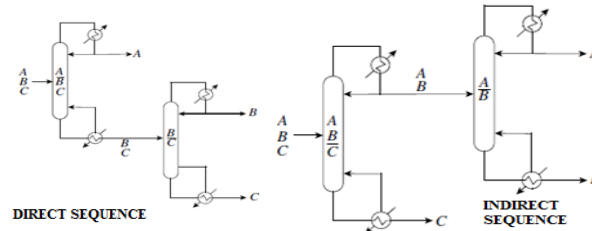
Figure 1.3 Direct and Indirect Sequence.

The heuristics [5] are based on observations made in many problems and attempt to generalize the observations. They can be summarized by the following four:
Heuristic 1.

Separations where the relative volatility of the key components is close to unity or that exhibit azeotropic behaviour should be performed in the absence of non key components. In other words, does the most difficult separation at last.
Heuristic 2.

Sequences that remove the lightest components alone one by one in column overheads should be favoured. In other words, favour the direct sequence.
Heuristic 3.

A component composing a large fraction of the feed should be removed first.
Heuristic 4.

Favour splits in which the molar flow between top and bottom products in individual columns is as near equal as possible.

Sequencing involving a four component organic mixture is given below,
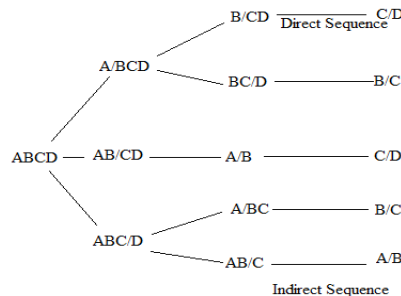
Figure 1.4 Alternative sequences for the separation of a four product mixture.

METHODOLOGY
Determination Of Distribution Coefficient:
Distribution co efficient (K) was determined using the Antoine's equation [5]

$$K_i = \frac{1}{P} e^{\left[A_i - \frac{B_i}{C_i + T}\right]} \qquad (2.1.1)$$

Where,

P = system operating pressure in bar.
T = guess temperature (bubble or dew point temperature).
A, B, C = Antoine's constants at fixed temperature and pressure for the respective components.

Bubble Point Calculations:
Bubble point was calculated using the flash calculation condition [5],

$$\sum Z_i * K_i = 1 \qquad\qquad (2.1.2)$$

Dew Point Calculation:
Dew point was calculated using the condition [5],

$$\sum \frac{Z_i}{K_i} = 1 \qquad\qquad (2.1.3)$$

Where,

Z_i = the feed composition of each of the components in the organic mixture.
The Bubble point (eqn. 3.1.2) and Dew point (eqn. 3.1.3) temperature was estimated by satisfying the above two conditions respectively and K was determined from eqn.3.1.1.

Calculation Of Minimum Number Of Stages:
Minimum number of stages was calculated using Fenske's Equation [3],

$$N_{min} = \frac{\log[\frac{r_{L,D}}{1-r_{L,D}} \cdot \frac{r_{H,B}}{1-r_{H,B}}]}{\log \alpha_{LH}} \qquad\qquad (2.2.1)$$

Where,

$\alpha_{L,H}$ = relative volatility between the light and heavy key component
r_{LD} = the percentage recovery of light key in the distillate
r_{HB} = the percentage recovery of heavy key in the bottoms.

Relative Volatility:
Relative volatility was calculated by taking the ratios of the distribution co efficient.

i.e. $\alpha = \frac{K_i}{K_j}$,   using Raoult's Law.   (2.2.2)

Where,

α = relative volatility of all the components in the organic mixture.
K_j = the reference component (the heaviest component in the organic mixture).

Bottoms And Distillate Composition:
The distribution of components was determined by using the equations

$$d_i = \frac{\alpha_{i,j}{}^{Nmin} f_i(\frac{d_j}{b_j})}{1 + \alpha_{i,j}{}^{Nmin}(\frac{d_j}{b_j})} \qquad\qquad (2.2.3)$$

$$b_i = \frac{f_i}{1 + \alpha_{i,j}{}^{Nmin}(\frac{d_j}{b_j})} \qquad\qquad (2.2.4)$$

The equations were obtained from rearranging and substituting in Fenske's equation [3] [5].
The mole fractions were then determined using the equations,

$$x_{id} = \frac{x_{id}}{\sum x_{id}} \qquad\qquad (2.2.5)$$

$$x_{ib} = \frac{x_{ib}}{\sum x_{ib}} \qquad\qquad (2.2.6)$$

Determination Of Minimum Reflux Ratio:
Underwood equations were used at Minimum reflux conditions to determine the minimum reflux ratio, using two equations.

Underwood Equation no. 1:

$$\sum_{i=1}^{NC} \frac{\alpha_{ij*}\, x_{i,f}}{\alpha_{ij} - \theta} = 1 - q \qquad (2.3.1)$$

Where,

$\alpha_{i,j}$ = relative volatility, $x_{i,f}$ = mole fraction of component in the feed
θ = root of the equation, q = feed condition (saturated feed = 1)
NC = number of component.

Here, the value of θ was determined such that, it satisfies the condition of eqn. 2.3.1. This value of θ was used in the second Underwood equation to determine R_{min} (minimum reflux ratio).

Underwood Equation no 2:

$$\sum_{i=1}^{NC} \alpha_{ij}*(\frac{x_{id}}{\alpha_{ij} - \theta}) = R_{min} + 1 \qquad (2.3.2)$$

Where,

X_{id} = mole fraction of components in the distillate of the column.

Theoretical Number Of Stages:
Theoretical stages was determined using Gilliland equation [8],

$$\frac{(N - N_{min})}{N+1} = 1 - e^{\left[\left(\frac{1 + \frac{54.4(R - R_{min})}{(R+1)}}{11 + \frac{117.2(R - R_{min})}{(R+1)}} \right) \left(\frac{\frac{(R - R_{min})}{(R+1)} - 1}{[\frac{(R - R_{min})}{(R+1)}]^{0.5}} \right) \right]}$$

$$(2.4.1)$$

Where,

N = actual number of theoretical stages,
R_{min} = minimum reflux ratio
N_{min} = minimum number of theoretical stages,
R = actual reflux ratio

Gilliland represented the correlation graphically with $\frac{(N - N_{min})}{N+1}$ as y-axis and $\frac{(R - R_{min})}{(R+1)}$ as x-axis. The equation 2.4.1 thus was represented algebraically as:

$$Y = (0.2788 - 1.3154 * X + 0.4114 X^{0.2910} + 0.8268 * \ln X + 0.9020 \ln\left(X + \left(\frac{1}{X} \right) \right) \qquad (2.4.2)$$

Where,

X, Y are co relating parameters

i.e. $X = \frac{(R - R_{min})}{(R+1)}$ $Y = \frac{(N - N_{min})}{N+1}$ \qquad (2.4.3), (2.4.4)

Estimation Of Physical Properties:
The physical properties like mass flow rate in the vapour phase and liquid phase, the density in vapour and liquid phase, surface tension, viscosity of the components in the bottom and the distillate were determined with respect to mole fractions obtained and its corresponding mass fractions.

Determination Of Column Efficiency:
Efficiency of the column was estimated using the equation,

$$E_O = 0.542 - 0.285 \log (\alpha_{LH}.\mu_L) \qquad (2.5.1)$$

Where,

E_O = overall stage efficiency ($0 < E_O < 1$)

α_{LH} = relative volatility between the key components

μL = viscosity of the feed at average column conditions ($mN \cdot s \cdot m^{-2} = cP$)

DETERMINATION OF COLUMN HEIGHT:
The height of the distillation column is calculated using the formula [5],

$$H = C (N_R - 1) + C_T \qquad (2.5.2)$$

Where,

H = Height of the column

C = Plate Spacing (m)

C_T = Allowance

Determination Of The Column Diameter:
The flow factor was calculated as well as the tray space and the column was considered to be operated at 85% of the flooding capacity. The column down-comer, net, and active areas were specified as well as the diameter of the column at 85% of the flooding velocity [5] [17] [18].

Initially the liquid and the vapour flow rate above and below the feed were determined, followed by the determination of liquid-vapour flow parameter [5]

$$F_{L,V} = \left(\frac{M_L L}{M_V V}\right) \left(\frac{\rho_V}{\rho_L}\right)^{0.5} \qquad (2.5.3)$$

The vapour flooding velocity is determined assuming a foaming fraction of 0.9 and with the terminal velocity parameter K_T [5]

$$v_T = 0.9 K_T \left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{0.5} \qquad (2.5.4)$$

Where,

L = liquid molar flow rate ($kmol \cdot s^{-1}$),

V = vapor molar flow rate ($kmol \cdot s^{-1}$)

$F_{L,V}$ = liquid vapour flow parameter,

M_L = liquid molar mass, M_V = vapour molar mass,

ρ_V = vapor density, ρ_L = liquid density ($kg \cdot m^{-3}$).

To obtain the column diameter, an allowance must be made for down comer area (say 10%), and the vapor velocity

$$Diameter = \left(\frac{4 M_V V}{0.9 * 0.8 * \pi * \rho_V * v_T}\right)^{0.5} \qquad (2.5.5)$$

The diameter was then determined for the top and bottom of the distillation column with respect to its flow rate parameters and terminal velocity parameters at the top and bottom of the column respectively.

Distillation Column Sequencing:
Distillation column sequencing was done with reference to certain heuristics [5] and the best sequence was determined by estimation of the least vapour load at 100 percent recovery condition. The number of sequences was obtained from the formula based on the number of products P.

$$N_s = \frac{(2(P-1))!}{P!(P-1)!}$$ (2.6.1)

The possible sequences thus obtained for the given five component organic mixture A,B,C,D,E with A being the lightest component and E being the heaviest component.

Table 2.1 Sequences for the given five component organic mixture (ABCDE)

No.		SEQUENCES		
1	AB/CDE	A/B	C/DE	D/E
2	A/BCDE	B/CDE	C/D	D/E
3	A/BCDE	BC/D	B/C	D/E
4	AB/CDE	CD/E	A/B	C/D
5	ABC/DE	A/BC	B/C	D/E
6	A/BCDE	B/CDE	CD/E	C/D
7	A/BCDE	BCD/E	BC/D	C/D
8	ABC/DE	AB/C	B/C	D/E
9	ABCD/E	A/BCD	B/CD	C/D
10	ABCD/E	AB/CD	A/B	C/D
11	A/BCDE	BCD/E	BC/D	B/C
12	ABCD/E	A/BCD	BC/D	B/C
13	ABCD/E	ABC/D	A/BC	B/C
14	ABCD/E	ABC/D	AB/C	A/B

RESULTS AND DISCUSSIONS
Organic Mixture Details:
Following case study was chosen [5]

Table 3.1 Organic Mixture details

COMPONENT	FORMULA	FEED
ETHANE	C_2H_6	5
PROPANE	C_3H_8	25
n-BUTANE	C_4H_{10}	30
n-PENTANE	C_5H_{12}	20
n-Hexane	C_6H_{14}	20

The above mixture has to be separated by distillation such that 95% of the propane is recovered in the distillate and 90% of the butane is recovered in the bottoms (for a column operating at 10 bar).

Determination Of Distribution Coefficient:
For determining distribution coefficient Antoine's equation was used and the following values of Antoine's Constants were chosen [5].

Table 3.2 Antoine's Constants

A	B	C
9.0435	1511.4	-17.16
9.1058	1872.5	-25.16
9.058	2154.9	-34.42
9.2131	2477.1	-39.94
9.2164	2697.6	-49.78

Bubble Point Calculation:
Bubble point was calculated using the flash calculation condition [5],

$$\sum Z_i * K_i = 1$$

(3.2.1)

$$K = \frac{1}{10}\exp\left(9.0435 - \left(\frac{1511.4}{(-17.16+T)}\right)\right)$$ (3.2.2)

Table 3.3 Distribution coefficients for given components

z_i	K_i (T=327.88 K)	$z_i * K_i$
0.05	6.50248	0.3251
0.25	1.84356	0.4608
0.3	0.55161	0.1655
0.2	0.1825	0.0365
0.2	0.06102	0.0122

$$\sum \quad 1.0001$$

From table 3.3 the Boiling Point was found to be 327.88 K.

Dew Point Calculation:

Dew point was calculated using the condition [5],

$$\sum \frac{Z_i}{K_i} = 1 \qquad\qquad (3.2.3)$$

Table 3.4 Distribution coefficients for given components

z_i	K_i (T=359.7599 K)
0.05	10.2713
0.25	3.343
0.3	1.14
0.2	0.533
0.2	0.1671

From table 3.4 the Dew Point was found to be 359.7599 K .

Determination Of Relative Volatility:

Relative Volatility of components was calculated using the distribution coefficients with the last component taken as the reference component.

$$A = \frac{0.55161}{0.06102} = 9.0396$$

Table 3.5 Relative volatilities of components in the organic mixture

ith component	jth component	$\alpha_{i/heptane}$
Ethane	n-Hexane	106.563
Propane	n-Hexane	30.212
Butane	n-Hexane	9.0396
n-Pentane	n-Hexane	2.9908
n-Hexane	n-Hexane	1

From the above table relative volatility between light and heavy key was found to be 3.37

Therefore, from Fenske's Equation the minimum number of stages was found to be,

$$N_{min} = \log[\frac{\left(\frac{0.95}{1-0.95} * \left(\frac{0.9}{1-0.9}\right)\right]}{\log 3.342}, = 4.27$$

Bottoms And Distillate Composition:

Heavy key was taken as the reference component,

$$\frac{D_h}{B_h} = \frac{1-0.9}{0.9} = 0.111 \qquad\qquad (3.4.1)$$

$$D_i = \frac{0.05*(0.1111)\alpha^{4.27}}{1+(0.1111)\alpha^{4.27}} \qquad (3.4.2)$$

$D_i = 4.9987$

$$B_i = \frac{0.05}{1+(0.1111)\alpha^{4.27}} \qquad (3.4.3)$$

$B_i = 0.002$

$$x_{id} = \frac{4.9987}{31.7686} \qquad (3.4.4)$$

$$x_{ib} = 0 \qquad (3.4.5)$$

Table 3.6 Distribution of Components

Components	Di (kmol/h)	Bi (kmol/h)	X_{di}	X_{bi}
Ethane	4.9987	0.0012	0.1573	0
Propane	23.75	1.25	0.7475	0.0183
Butane	3	27.003	0.0944	0.3957
Pentane	0.0195	19.9805	0	0.2928
Hexane	0	19.9998	0.0	0.29312
Σ	31.7686	68.2309	0.9999	0.9999

Determination Of Minimum Reflux Ratio:
First Underwood Equation was used to determine θ (root of the equation)

Table 3.7 Solution for The Root Of The Equation.

X_{fi}	α_{ij}	$\alpha_{ij}*X_{fi}$	$\alpha_{ij}*X_{fi}/ \alpha_{ij}- \theta$
0.05	106.563	5.32815	0.05799
0.25	30.212	7.553	0.4868
0.3	9.0396	2.71188	-0.4792
0.2	2.9908	0.59816	-0.0511
0.2	1	0.2	-0.0146

From the above table ,the value of θ, satisfying the conditions of the first Underwood Equation was found to be 14.6963

Table 3.8 Solution for the second Underwood equation

X_{di}	α_{ij}	$\alpha_{ij}*X_{di}$	$\alpha_{ij}*X_{di}/\alpha_{ij}-\theta$
0.1573	106.563	16.7623	0.18246
0.7475	30.212	22.5834	1.4555
0.0944	9.0396	0.8533	-0.1508
0	2.9908	0	0
0	1	0	0
			Σ =1.4871

Determination Of Theoretical Number Of Stages:
Theoretical number of stages was determined using Gilliland's Equation,

$$X = \frac{(0.5358-0.4871)}{(0.4871+1)} = 0.0317 \qquad (3.6.1)$$

$$Y = (0.2788 - 1.3154*X + 0.4114*0.0317^{0.2910} + 0.8268*\ln 0.0317 + 0.9020 \ln(0.0317 \left(\frac{1}{0.0317}\right))$$

$$(3.6.2)$$

$$Y = 0.6482$$

Theoretical stages (N)

$$0.6482 = \frac{(N - N_{min})}{N+1} \ , \quad N = 14 \text{ stages.}$$

Determination Of Column Efficiency:

Efficiency of the column was estimated using the equation,

$E_O = 0.542 - 0.285 \log (3.37*0.0275) = 0.8378$ 　　　(3.7.1)

Number of real trays, $N_R = 14/0.8378 = 17$ stages

$$(3.7.2)$$

Estimation Of Physical Properties:

For the organic mixtures, the mole fractions and mass fractions of the components in the liquid and vapour phase are estimated and tabulated as show in the table 4.9.

Table 4.9 Physical properties estimated using

DISTILLATE	
liquid molar flowrate	43.18125 Kg\Kmol
vapor molar flowrate	37.69475Kg\Kmol
vapor density	16.0525Kg\m³
liquid density	383.894Kg\m³
surface tension	4.5245mN\m²
BOTTOMS	
liquid molar flowrate	69.3845Kg\Kmol
vapor molar flowrate	53.005Kg\Kmol
vapor density	25.7935kg\m³
liquid density	393.566kg\m³
surface tension	3.8061N\m²

Determination Of the Column Height:

The height of the column was estimated using the equation, the plate spacing was taken as 0.45m and 4m allowance at the top [5] [18].

$$\text{Height} = 0.45(17 - 1) + 4 = 8.6515\text{m} \qquad (3.7.3)$$

Determination Of The Column Diameter:

The flow factor was calculated as well as the tray space and the column was considered to be operated at 85% of the flooding capacity. The column down-comer, net, and active areas were specified as well as the diameter of the column at 85% of the flooding velocity [5] [18].

The distillate flow rate = 32.6461 kmol/hr

Taking mass balance on the top of the column resulted in,

$$V_{top} = D(R + 1) = 49.1682 \text{ kmol/hr} \qquad (3.7.4)$$

$$L_{top} = R*D = 18.1744 \text{ kmol/hr} \qquad (3.7.5)$$

Feed of 100 kmol/hr was a saturated liquid therefore, the liquid flow rate at the bottom,

L_{bottom} = 118.1744 kmol/hr   (3.7.6)

 The bottom flow rate = 67.3539 kmol/hr

V_{bottom}=50.82 kmol/hr

The Liquid Flow Parameter:
At the top of the column:
$$F_{L,V} = \left(\frac{43.18125*18.1744}{37.69475*49.1682}\right)\left(\frac{16.0525}{383.894}\right)^{0.5}$$

$= 0.0864$ (3.7.7)

At the bottom of the column:

$$F_{L,V}' = \left(\frac{69.4825*18.1744}{53.005*50.8205}\right)\left(\frac{25.7935}{393.566}\right)^{0.5}$$

$= 0.779$ (3.7.8)

The Velocity Parameter:
At the top of the column:

$$K_T = \left(\frac{4.5245}{20}\right)^{0.5} e^{\left(\substack{-2.979-0.717\ln(0.0864)-0.0865(\ln 0.0864)^2+0.997\ln 6.25 \\ -0.07973\ln 0.0864*\ln 6.25+0.256*\ln 6.25}\right)}$$
(3.7.9)
  $K_T = 0.0591$ m/s

 At The Bottom Of The Column:

$$K_T' = \left(\frac{3.8061}{20}\right)^{0.5} e^{\left(\substack{-2.979-0.717\ln(0.779)-0.0865(\ln 0.779)^2+0.997\ln 6.25 \\ -0.07973\ln 0.779*\ln 6.25+0.256*\ln 6.25}\right)}$$
                                         (3.7.10)
K_T' = 0.02268 m/s

Vapour Flooding Velocity:
At the top of the column:

$$V_T = 0.9*0.0591*\left(\frac{383.894-16.0525}{16.0525}\right)^{0.5} = 0.2546 \text{ m/s}$$
(3.7.11)
At the bottom of the column:

$$V_{Bottom} = 0.9*0.02268*\left(\frac{393.566-25.7935}{25.7935}\right)^{0.5} = 0.0771 \text{ m/s}$$
(3.7.12)

Diameter:
At the top of the column:

$$Dia_T = \left(\frac{4*37.6947*50/3600}{0.9*0.8*16.0525*0.2546*\pi}\right)^{0.5}$$
$= 0.4759$m.   (3.7.13)

At the bottom of the column :

$$Dia_B = \left(\frac{4*53.005*50/3600}{0.9*0.8*25.7935*0.0771*\pi} \right)^{0.5}$$
$$= 0.8091 \text{ m} \qquad\qquad (3.7.14)$$

Feed Tray Location:
The feed tray location is obtained from Kirkbride (1994) empirical equation [5],

$$N_R + N_S = 17 \text{ and } N_R = N_S*0.62 \qquad (3.7.15, 3.7.16)$$

$$N_S = 11^{th} \text{ tray}$$

Where,

> N_R = trays in the Rectifying Section.
> N_S = trays in the Stripping Section.

Distillation Column Sequencing:
The procedure carried out for the design of a distillation column was used in the estimation of the vapour flowrate from each distillation column within one particular sequence (around four separate distillation columns connected depending on to way of operation sequence) carried out at 100% recovery conditions. The vapour flowrate from each column in a particular sequence was added to obtain 'the total vapour flowrate,' against which the best one was chosen depending on the one with the least total vapour load.

The sequences, along with their total vapour loads have been ranked and tabulated and the best sequence was obtained.

$$V = D (1+R)$$

Where,

> V = Vapour load (kmol/hr), D = Distillate flowrate (kmol/hr), R = Reflux ratio.

Table 4.10 Sequences for the separation of alkanes fixed at 10bar pressure and relative volatilities fixed by feed to sequence

RANK ORDER	VAPOR RATE(Kmol/hr)	SEQUENCES			
1	162.4085	AB/CDE	C/DE	A/B	D/E
2	166.263	A/BCDE	B/CDE	C/D	D/E
3	188.8845	A/BCDE	BC/D	B/C	D/E
4	191.2606	AB/CDE	CD/E	A/B	C/D
5	192.7765	ABC/DE	A/BC	B/C	D/E
6	195.1151	A/BCDE	B/CDE	CD/E	C/D
7	220.8125	A/BCDE	BCD/E	BC/D	C/D
8	226.28	ABC/DE	AB/C	B/C	D/E
9	229.3275	ABCD/E	A/BCD	B/CD	C/D
10	229.3275	ABCD/E	AB/CD	A/B	C/D
11	245.103	A/BCDE	BCD/E	BC/D	B/C
12	247.3929	ABCD/E	A/BCD	BC/D	B/C
13	250.9011	ABCD/E	ABC/D	A/BC	B/C
14	257.792	ABCD/E	ABC/D	AB/C	A/B

From the table 3.10, the best sequence for the five component mixture thus obtained was AB/CDE→ C/DE → A/B → D/E with, total vapour load = 162.4085 kmol/hr.

CONCLUSIONS
For the given organic mixture of ethane, propane, butane, n-pentane and n-hexane with Propane being the light key component and Butane being the heavy key component, Fenske's Equation was used to calculate minimum number of stages and was found to be 4.2. The Underwood equations gave a minimum reflux ratio of 0.4871 and actual reflux ratio of 0.5358. In calculating distribution coefficient simple equation like Antoine's' Equation was used along with Raoult's Law for the calculation of relative volatility. It was found that 95% of propane (23.75 kmol/hr) was recovered in the distillate and 90% of butane (27.003 kmol/hr) was recovered in the bottoms. For the given organic mixture a distillation column was designed. The design calculation gave the height to be, 8.65m and, top diameter of 0.4759m and bottom diameter of 0.8091m.

An attempt was made to understand the concept of distillation column sequencing. Based on the relative volatility fixed at feed to the column for 100% recovery of the distillate. The best sequence was found to be AB/CDE → C/DE → A/B → D/E With the total vapour load being 162.4085 kmol/hr.

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