INTERACTIVE M-FILE ALGORITHM FOR ESTIMATING NUMBER OF PLATES AT TOTAL REFLUX IN A DISTILLATION COLUMN

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ABSTRACT

This paper presents an interactive M-file algorithm capable of running in a MATLAB environment, which can estimate the number of theoretical plates a distillation column ought to contain at total reflux to efficiently separate a multicomponent mixture into their individual components. Fenske's model was used to achieve the estimation at total reflux, and six feed variations for the multicomponent mixture of propane, iso-butane, n-butane, iso-pentane and n-pentane were used as case studies. The first three feed variation have iso-butane and n-butane as the light and heavy key respectively while the last three feed variation have iso-pentane and n-pentane as the light and heavy key respectively. 2.324, 2.321, 2.321, 2.775, 2.718 and 2.691 average relative volatilities, condenser temperatures of 324K, 325K, 325K, 357K, 359K and 360K, reboiler temperatures of 369K, 371K, 372K, 387K, 387K and 387K obtained for the six feed variations respectively when applied in Fenske's model, gave a minimum of 6.62, 6.66, 6.63, 6.57, 6.72 and 6.77 plates as the number of theoretical plates required by the column for optimum separation of the components in each feed variation. This method is simple, robust and saves time.

Keywords: M-file Algorithm, Fenske's model, Plates, Feed variation, Total reflux

1.0 INTRODUCTION

Fenske's model is an approximate method that has been widely used for preliminary design and optimization of simple distillation column's processes [1]. According to [2], it calculates the number of plates for a given separation based on total reflux condition.

Although this method can be applied readily by manual calculation, computer calculations are preferred. The Fenske's model is included in most computer-aided process design programs [1]. It relies on certain simplifying assumptions, such as

constant relative volatilities and constant molar overflow along each column section [3]. In Fenske's model, the relative volatility (α) is an important parameter [2]. The total reflux condition can be achieved by operating the column at finite feed and product output with a very high reflux rate or by operating it with no further input of feed and no withdrawal of products [1]. The column considered here is a conventional simple column, which has the following features: a single feed, an overhead product, a liquid bottom product, multi-plate column with one condenser at the top and one reboiler at the bottom. An important assumption of this method is related to the vapour-liquid equilibrium coefficient or K-value [4]. The derivation was based on the assumptions that the stages are equilibrium stages [5]. The concept of key components was adopted in the work of [2], which allows multicomponent separations to be treated as separations of simple binary mixtures.

The objectives of this paper are:

a. To obtain an estimate of the number of theoretical plates in a distillation column using Fenske's model.
b. To develop a computer-based M-file algorithm capable of producing converged solutions to the computed problem.
c. To ensure the algorithm is interactive with its end-user(s) by being simple, robust, fast and modifiable.

2.0 THEORETICAL ANALYSIS

It is obvious that good design requires good data especially so with multicomponent calculations [6]. Vapour-liquid equilibrium is calculated by Antoine equation [7]:

$$log P^{o}_{vap} = A - \frac{B}{T+C} \qquad (1)$$

P_{vap}= vapour pressure of the component
A, B, C = Antoine constants
T = absolute temperature in Kelvin
Table 1 displays Antoine constants obtained from [4]:

Table 1: Antoine constants for the system $C_3 – C_5$

Components	A	B	C
Propane	15.7260	1872.46	-25.16
Iso-butane	15.5381	2032.73	-33.15
n-butane	15.6782	2154.90	-34.42
Iso-pentane	15.6338	2348.67	-40.05
n-pentane	15.8333	2477.07	-39.94

For equilibrium relationship:

$$Ki = Pi/P \qquad (2)$$

Where: Pi=vapour pressure of component i
P = total column's pressure
The relative volatility, defined by the ratio of K-values of any two components (i and j) is assumed to be constant throughout the whole column [1].

$$\alpha_{i,j} = K_i/K_j \qquad (3)$$

K = vapour-liquid equilibrium or distribution coefficient (K-value)
The relative volatilities may vary somewhat with composition and temperature inside a column, so it is necessary to use average values [8]. The most commonly used approximation for which the average α is computed as the geometric mean value according to [8], [1], [9], and [10] is:

$$\alpha_{av} = (\alpha_{top} + \alpha_{bot})/2 \qquad (4)$$

Where: α_{av} = average relative volatility for a component.
α_{top}, α_{bot} = relative volatilities of the component in the top and bottom of the column.

Dew points and bubble points can be calculated from the vapour-liquid equilibrium for the system. In terms of equilibrium constants, they are defined by:

Bubble point: $\sum y_i = \sum(K_i x_i) = 1.0$ (5)

Dew point:

$\sum x_i = \sum(y_i/K_i) = 1.0$ (6)

For multicomponent mixtures, the temperature that satisfies these equations, must be found by iteration [4]. The Fenske equation for a multi-component mixture by [2] is:

$$N_{min} = \frac{(\log(x_{LK}/x_{HK})_d(x_{HK}/x_{LK})_b)}{(log\alpha_{av,LK})} \quad (7)$$

N_{min} = minimum number of plates
$(x_{LK})_d$ = mole fraction of the light key in the distillate
$(x_{HK})_d$ = mole fraction of the heavy key in the distillate
$(x_{LK})_b$ = mole fraction of light key in the bottom
$(x_{HK})_b$ = mole fraction of the heavy key in the bottom
$\alpha_{av,Lk}$ = average relative volatility of the light key component

By defining key components (LK and HK) in the Fenske equation, the problem of determining Nmin for a given separation becomes relatively simple regardless of how many components are contained in the mixture. The simplicity of the Fenske method is an advantage for predicting product compositions, especially for a mixture involving a large number of components, such as crude oil distillation or other separations in the petroleum industry.

3. DESIGN METHODOLOGY:

The general program design steps for obtaining solutions for each of the estimated variables based on [11] are:

a. State the design problem that requires a solution.
b. Define the input and output variables required to write the M-file.
c. Design the program algorithm.
d. Develop a flowchart for the algorithm.
e. Convert the algorithm into MATLAB M-file statements.
f. Test the designed M-file program to ensure it is working properly and error-free, thereby producing converged solution to the computed problem.

Design Assumptions

a. Pressure is assumed to be constant throughout the whole column.
b. Stages are equilibrium stages.
c. The feed is assumed to be mostly liquid at boiling point.
d. Relative volatility is assumed to be constant at different temperature and pressure.

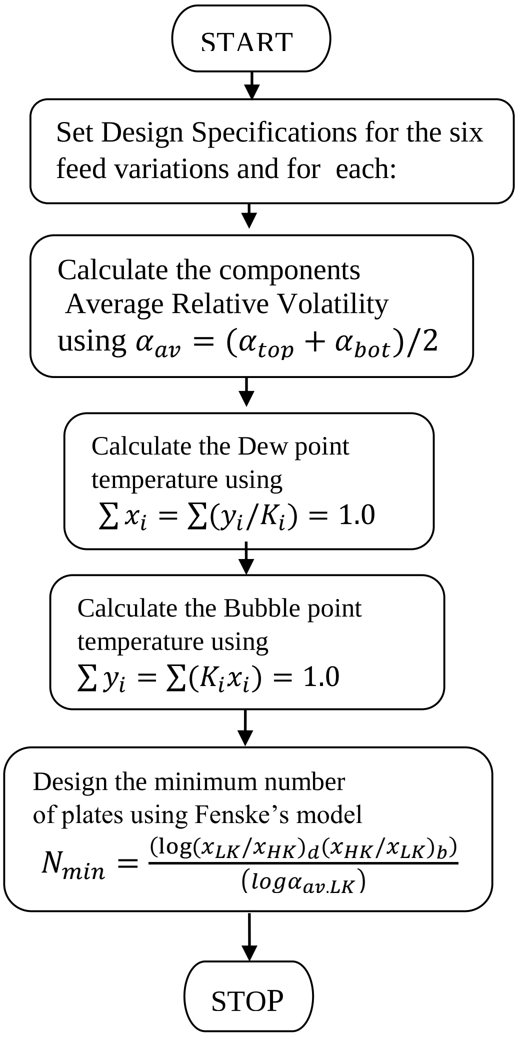


Figure 1: Conceptual flowchart for the required general processes.

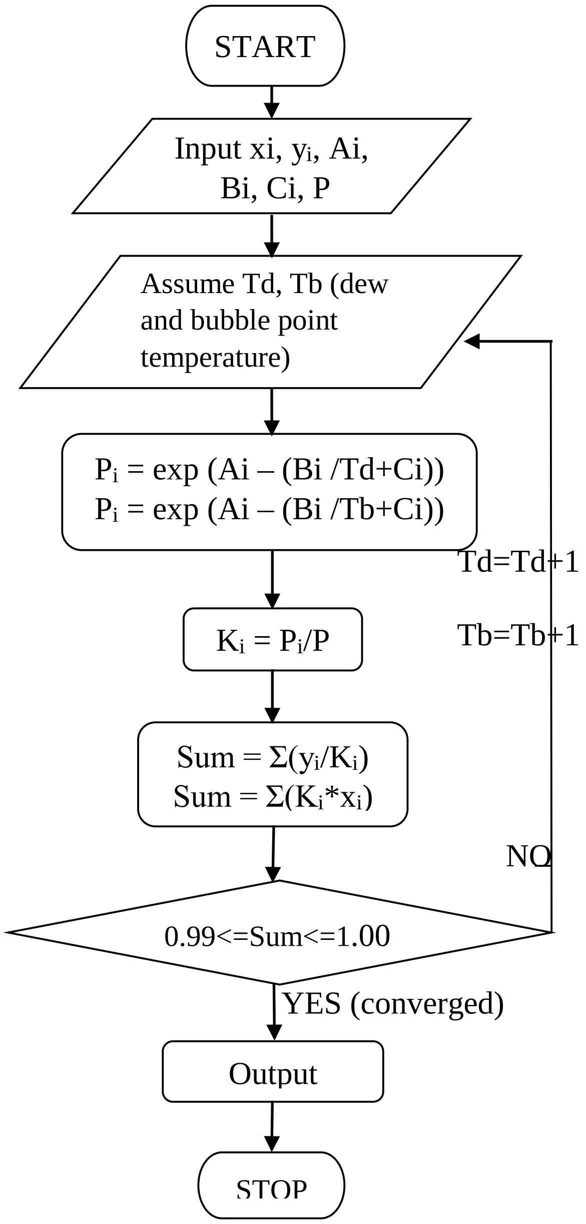


Figure 2: Flowchart algorithm for dew and bubble point temperatures.

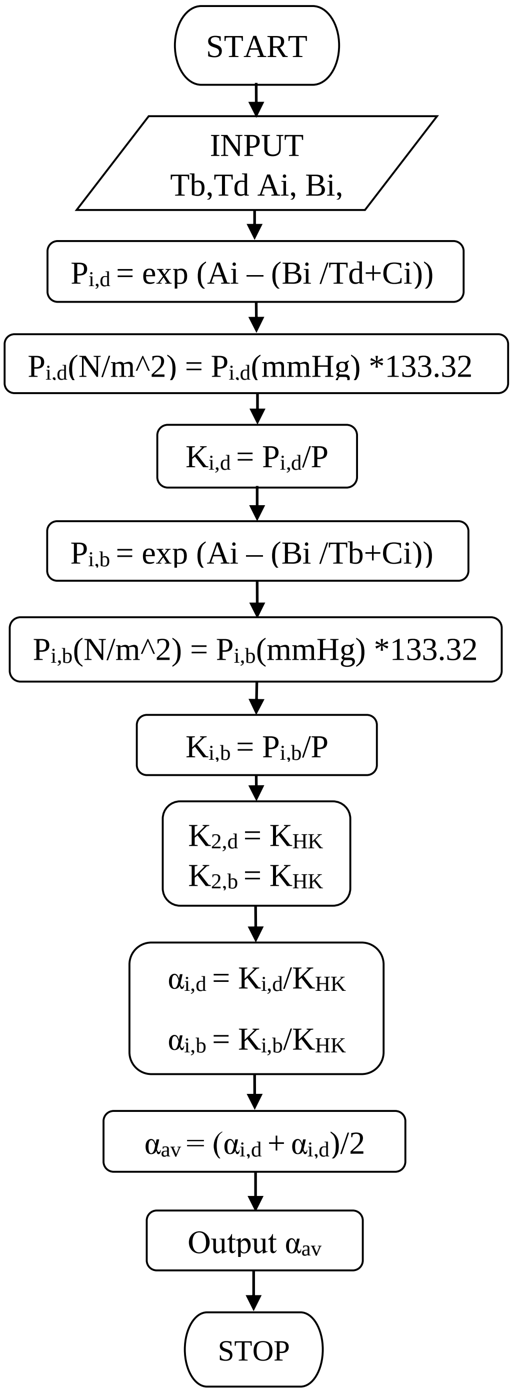
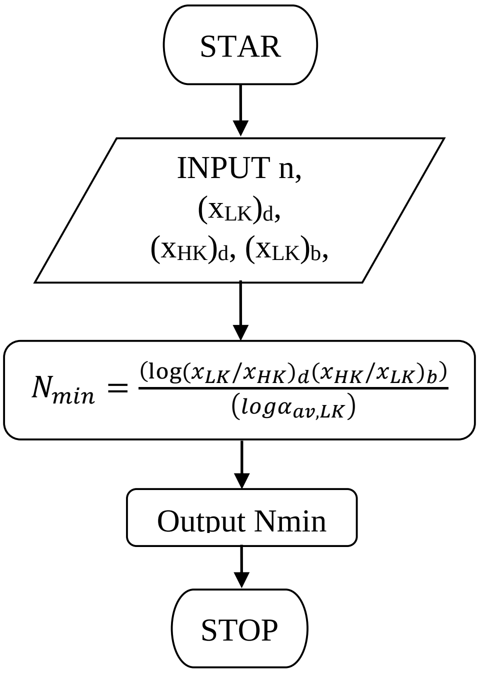


Figure 3: Flowchart algorithm for determining average relative volatility



4. RESULTS AND DISCUSSION

At a column's pressure of 800kN/m^2 and applying the product compositions for the six feed variations in [11] for which the compositions of their base feed variations are in Table 1 and 2, the M-file results obtained are displayed in this section:

Figure 4: Flowchart algorithm for solving Fenske's model

Table 2: Result for the first base feed variation

Feed	F (kmol/s)	x_f	D (kmol/s)	x_d	B (kmol/s)	x_b
C3	5	0.05	5	0.25	-	-
(LK) i-C4	15	0.15	14	0.70	1	0.013
(HK) n-C4	20	0.20	1	0.05	19	0.238
i-C5	35	0.35	-	-	35	0.437
n-C5	25	0.25	-	-	25	0.312
Sum :	100	1.00	20	1.00	80	1.00

Table 3: Result for the second base feed variation

FEED	F (kmol/s)	x_f	D (kmol/s)	x_d	B (kmol/s)	x_b
C3	5	0.05	5	0.067	-	-
i-C4	15	0.15	15	0.20	-	-
n-C4	20	0.20	20	0.267	-	-
(LK) i-C5	35	0.35	34	0.453	1	0.04
(HK) n-C5	25	0.25	1	0.013	24	0.96
Sum :	100	1.00	75	1.00	25	1.00

In Table 2, five feed components with total feed flow rate of 100kmol/s produced a total distillate flow rate of 20kmol/s and a total bottom flow rate of 80kmol/s.

In Table 3, five feed components with total feed flow rate of 100kmol/s produced a total distillate flow rate of 75kmol/s and a total bottom flow rate of 25kmol/s.

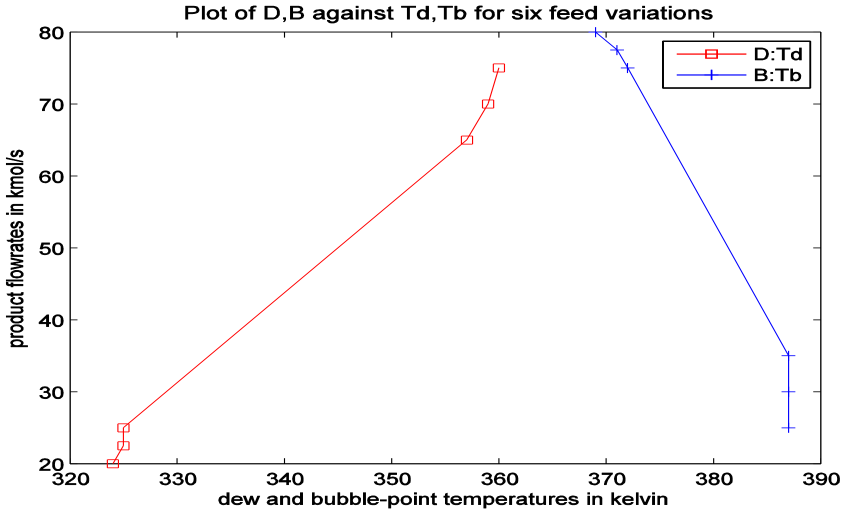


Figure 5: Plot of D and B against Td and Tb for the six feed variation

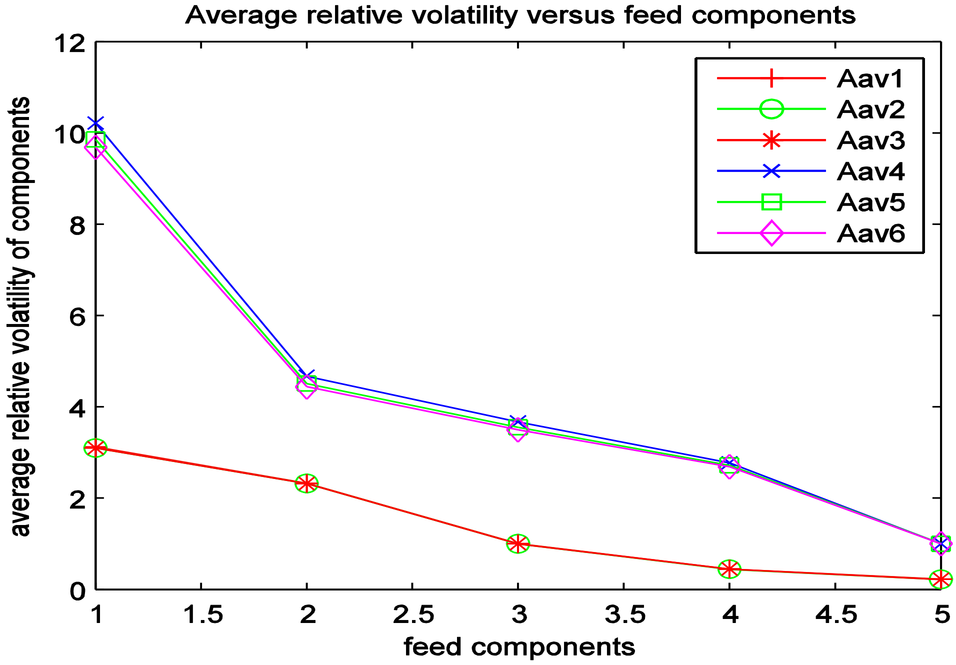


Figure 6: Average relative volatilities of components in the feed variations

The components in the fourth feed variation as seen in Figure 6 can be separated more easily in the distillation column than those of other feed variations due to its high average relative volatility based on [4].

Table 4: Result for the estimated dew point temperature

x_di	D (kmol/s)	Td (K)
For 5 cpts: x_d1	20	324
x_d2	22.5	325
x_d3	25	325
x_d4	65	357
x_d5	70	359
x_d6	75	360

The converged dew point temperatures (Tdi) of the column are shown in Table 4. The dew point temperature (Tdi) of the condenser increases as the distillate flowrate (Di) increases as seen in Figure 5.

Table 5: Result for the designed bubble point temperature

x_bi	B (kmol/s)	Tb (K)
5cpts: x_b1	80.0	369
x_b2	77.5	371
x_b3	75.0	372
x_b4	35.0	387
x_b5	30.0	387
x_b6	25.0	387

When the LK and HK for the first three variations (xb1, xb2, xb3) were i-C4 and n-C4 respectively from Table 5, the bubble point temperature for each feed variation increases. At the last three variations (xb4, xb5, xb6) where the LK and HK were i-C5 and n-C5 respectively, their bubble point temperature remained constant simply because of the presence of just one component (n-C5) in the bottoms. It still showed that as the bottom flowrate (Bi) decreases, the bubble point temperature increases as reflected in Figure 5. It correlates to other standardly designed column's bubble point temperature [4] and [9].

The flowchart algorithms in Figure 1 to 4 aided in developing a Matlab M-file algorithm capable of running error -free in a Matlab environment:

```
%%file name: minimum_stage.m
%this program calculates the theoretical number of stages required in a multicomponent distillation column using Fenske's model.
%Date:      Programmer:      Description of code change:
%=========  =========  =========
%26-12-2015 Okafor Blessing Original code
%%description of variables:

%X1 --distillate flowrate of LK in kmol/s
%X2 --distillate flowrate of HK in kmol/s
%X3 --bottom flowrate of LK in kmol/s
%X4 --bottom flowrate of HK in kmol/s
%Nmin --minimum number of plates
%A_LK --average relative volatility of Lk
%%prompt user for the input data
X1=input('enter distillate flowrate of light key,X1:');
X2=input('enter distillate flowrate of heavy key,X2:');
X3=input('enter bottom flowrate of light key,X3:');
X4=input('enter bottom flowrate of heavy key,X4:');
A_LK=input('enter average relative volatility of light key,A_LK:');
%Solve Fenske's model at total reflux condition:
D=X1/X2;
B=X4/X3;
Sum1=(log(D*B));
Sum2=(log(A_LK));
Nmin=(Sum1)/(Sum2);
```

```
fprintf('Nmin=%f/n',Nmin);
```

Table 6: Result for estimated number of plates at total reflux

Feed variation no	α_{avLk}	Nmin(plates)
1	2.324	6.62
2	2.321	6.66
3	2.321	6.63
4	2.775	6.57
5	2.718	6.72
6	2.691	6.77

From Table 6, a minimum of 7 plates approximately is required for the separation of the six feed variations in a distillation column. Its correlation with the dew and bubble point temperatures is shown in Figure 7 and 8 respectively.

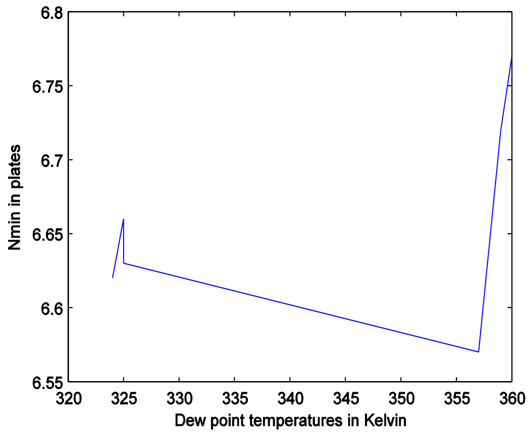


Figure 7: Nmin versus Td for the six feed variation

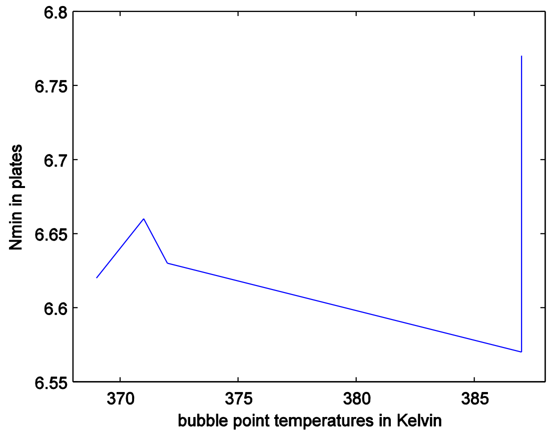


Figure 8: Nmin versus Tb for the six feed variation

CONCLUSION

With the aid of an interactive, simple, fast and robust Matlab M-file program for the Fenske's model, the estimated theoretical number of plates a distillation column will have to efficiently separate the six multicomponent feed variation are a minimum of 6.62, 6.66, 6.63, 6.57, 6.72, 6.77 plates each. This paper therefore concludes that from the results, an approximate of 7plates is required to separate the six feed variations at a condenser temperature of 324K, 325K, 325K, 357K, 359K and 360K respectively and a reboiler temperature of 369K, 371K, 372K, 387K, 387K, and 387K respectively. The M-File algorithm used is very interactive and can be modified to suit other user's needs. It is recommended that more feed variations be used as case-studies to compare with those used in this research for confirmation.

REFERENCES

[1] Seader, J. D. and Henley, E. J. (1998). *Separation process principles*, Wiley, New York.

[2] Fenske, M. R. (1932). *Fractionation of straight-run pennsylvania gasoline*, Journal of Industrial and engineering chemistry,Vol 24, Pp. 482-485.

[3] Khoury, F. M. (2005). *Multistage separation processes*, CRC Press, USA.

[4] Sinnott, R. and Towler, G. (2009). *Chemical engineering design*, 5th ed., Vol. 6, Coulson & Richardson's chemical engineering series, Butterworth-Heinemann, USA. Pp. 682-715.

[5] Thirumalesh, B. S. and Ramesh, V. (2015). *Case Study on Multicomponent Distillation and Distillation Column Sequencing*, International Journal of Engineering Sciences & Research Technology, Vol. 4, No. 8, Pp. 609-623.

[6] Gadzama, S. W., Ufomba, E. C., Okeugo, C. A., Nwachukwu, O. I., Agu, B. C., Ugwueze, O. S. and Roland, I. U. (2016). *Computer Aided Design of a Multi-Component Distillation Column using the FUG Shortcut Method*, Journal of Innovative Researches in Science and Engineering, Vol. 4, No. 3-1, Pp. 24-33.

[7] Rawia, S. H., Gurashi, A. G., Karama, B. A. and Musa, A. E. (2013). *A Short-cut Method for Designing Multi-component Fractionation Column*, Journal of Applied and industrial Sciences, Vol. 1, No. 3, Pp. 44-48.

[8] King, C. J. (1980). *Separation processes*, 2nd ed., McGraw-Hill Inc, New York.

[9] Kister, H. Z. (1992). *Distillation design analysis,* McGraw-Hill Inc, New York. Pp. 87-123.

[10] Van Winkle, M. (1967). *Distillation*, McGraw-Hill, New York. Pp. 525-526.

[11] Okafor, B. O. (2016). *Computer Aided Design and Simulation of a Plate Distillation Column*, M.Eng. Project Report, Department of Chemical Engineering, Chukwuemeka Odumegwu Ojukwu University, Uli, Nigeria.