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COMPUTER AIDED DESIGN OF A MULTI-COMPONENT DISTILLATION COLUMN FOR PROCESSING OF NIGERIAN BONNY LIGHT CRUDE OIL

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ABSTRACT

The design of the multi-component distillation column for processing of Bonny light crude is presented using advanced process simulation software (Aspen Hysys). The steady state design models were developed from Mesh equations and were used to obtain the design parameters based on the principle of conservation of mass and energy. The design parameters were column diameter, column cross sectional area, height of the column, downcomer area, hole area, weir length, wet area and tray spacing. The equations developed are capable of predicting compositions, partial pressures and temperature of the components of interest from the mixtures of crude oil. The accuracy of the design parameters were ascertained by comparing predicted results with literature data of a distillation unit. The simulation of the design models were performed using Aspen Hysys to obtain optimum values of the most significant variables/parameters (column diameters 1.558m, column height 17.048m, cross section area 1.907m^2, downcomer area 0.229m^2, tray spacing 0.5m, weir length 1.200m, hole area 0.191m^2 and wet area 1.678m^2). The result obtained from the steady state simulation shows that the feed flow rate, temperature and pressure influence the efficiency of the distillation column.

Keywords: Computer aided design, Multi-component distillation, Crude oil.

1. INTRODUCTION

The separation of liquid mixture into their several components is one of the major operations in chemical/petrochemical industries and distillation is perhaps the most widely used method of achieving it Onifade [1]. Approximately 95% of all liquid separations are carried out by distillation processes. This exceptional role played by distillation is founded on the fact that distillation is the only separation technique that is capable to fractionate a fluid mixture into its pure constituents and accounts for 3% of global energy consumption [2].

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Distillation is the oldest separation process and the most widely used unit operations in the industry. It involves the separation of a mixture based on the difference in the boiling point (or volatility) of its components [3]. The reason for the wide acceptance of distillation is that, from both kinetic and thermodynamics point of view, distillation offers advantages over other existing processes for the separation of fluid mixtures. (a) Distillation has the potential for high mass transfer rate because in general, in distillation there are no inert materials or solids present. (b) The thermodynamics efficiency for distillation is higher than the efficiency of most other available processes in the chemical industry [4]. Distillation column is made up of three distinct parts, namely; top, bottom and body. The top of the column is where the more volatile components are collected after condensation. Its products are called distillate [5]. The bottom of the column collects the less volatile component called the residue. The body of the column houses the trays and packings. It serves as the point where the feed is fed into the column. It has also the rectification section and the stripping section. It is at this place contact between the liquid and vapor is made [6]. Modern engineering practice is becoming largely dependent on computer and information technology. Computer Aided Design (CAD) is therefore used in the design, maintenance and operations of the plants [7-9]. Plants are generally made up of unit operation equipment, which are similar in functions and differ only in their duty or throughput [1]. However, Computer Aided Design of a multi-component distillation column achieves its objectives by the creation of two co-existing zones (Vapour and Liquid phase) at essentially the same temperature and pressure [10].

Akpa and Umuze [11] did a similar work, developing the model equations from MESH equations, but the model equations were first transformed into matrix, and then solved by matrix inversion using the MatLab Solver Program. This method has problem in obtaining the algebraic equations, which is transformed into matrix before solving with the matrix inversion using Matlab solver and it also have the problem of convergence. Pradhan [12] also did similar work on simulation and economic analysis of crude distillation unit, but the simulation was done using Aspen Plus which has different features from Aspen Hysys. Simulation of multicomponent reactive distillation column was carried out by Dagde and Harry [13]. The work was based on the production of Methyl Tertiary Butyl Ether (MTBE) and it was simulated using Microsoft Visual Basic Program. In Mathematical Modeling and Simulation of Multicomponent Distillation Column for Acetone Chloroform Methanol System by Olafadehan, et al. [14] an algorithm was developed for solving the program and it was simulated using MatLab. In this work, the design models for a multi-component distillation column are developed from the MESH equations based on the principle of conservation of mass and energy and simulated using Aspen Hysys simulation software, to obtain the necessary design parameters. This work investigates the impact of feed flow rates on the column and the impact of temperature and pressure on the column.

2. MODELS

2.1. Overall Stage Model

Figure 1 shows a schematic diagram of N trays in a distillation column. It also shows the direction of component I to and from stage N.

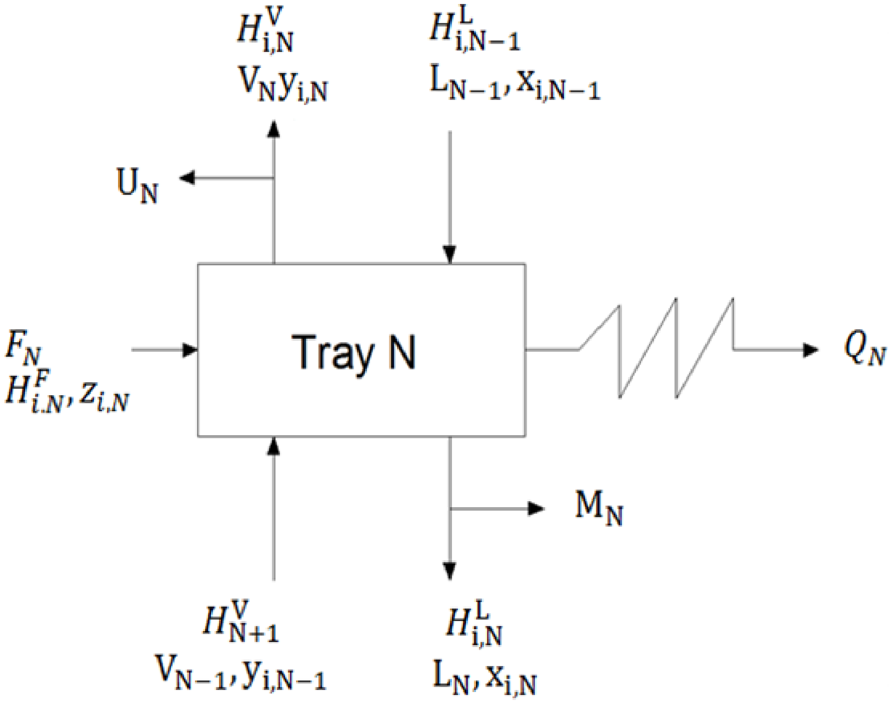

Figure-1. General Schematic representation of tray N

where; V_N is Vapour flow from the tray, V_{N-1} is Vapour flow into the tray from the tray below, L_N is Liquid flow from the tray, L_{N-1} is Liquid flow into the tray from the tray above, F is the Feed flow into the tray, Q is Heat flow into/removal from the tray, N is any tray numbered from the top of the column, Z is Mole fraction of component i in the feed stream, x is Mole fraction of component i in the liquid stream, y is Mole fraction of component i in the vapour stream, H^V is Specific Enthalpy vapour phase, H^L is Specific Enthalpy liquid phase, H^F is Specific Enthalpy feed (vapour + liquid).

2.2. Model Assumptions

In the derivation of the design models, the following assumptions are made:

- The feed stream is composed of four components
- The feed is introduced only at a point in the column
- The liquid and vapour flow rates are constant for all trays.

- Since the liquid and vapour flow rates in and out of each tray are constant them, the liquid and vapour hold- up in each tray will also be constant that is negligible vapour hold-up
- The overhead product is condensed in a total condenser
- The column is well lagged hence heat losses are negligible and for an ideal system heat of mixing is zero.
- For ideal systems of this kind, the molar heat of vaporization may be taken as constant and independent of the composition.

2.3. Material Balance Equation (M Equation)

Applying the conservative principle to the tray column in Fig. 1, gives the overall material balance as;

$$F_N Z_{i,N} + V_{N+1}Y_{i,N+1} + L_{N-1}X_{i,N-1} - V_N Y_{i,N} - L_N X_{i,N} - U_N Y_{i,N} - M_N X_{i,N} = 0\_\_\_\_\_(1)$$

Rearranging equation (1) gives;

$$F_N Z_{i,N} + V_{N+1}Y_{i,N+1} + L_{N-1}X_{i,N-1} = V_N Y_{i,N} + L_N X_{i,N} + U_N Y_{i,N} + M_N X_{i,N}\_\_\_\_\_\_(2)$$

Equation (2) is the general model equation that predicts the flow of component mass 'i' in and out of a given tray N. Rearranging equation (2) gives

$$F_N Z_{i,N} + V_{N+1}Y_{i,N+1} + L_{N-1}X_{i,N-1} - (L_N + M_N)X_{i,N} - (V_N + +U_N)Y_{i,N} = 0\_\_\_\_\_(3)$$

- **Equilibrium (Phase) Relationships (E Equation)**
- The k-value for the liquid and vapour phases of the ideal mixture is given by;

$$y_i = k_i x_i\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_(4)$$

- where; $k_i$is Phase equilibrium constant, For i = 1 to 5 which represents components as follows; 1 is Naphtha, 2 is Kerosene, 3 is Diesel, 4 is Automotive Gas Oil and 5 is the Residue
- **Summations of Mole Fraction (S Equation)**

$$\sum x_{i,N} = 1, \qquad \sum y_{i,N} = 1\_\_\_\_\_\_\_\_\_\_\_\_\_\_(5)$$

2.4. Heat/Energy Balance (H Equation)

Applying the conservative principle to the tray column in Fig. 1, gives the overall heat/energy balance as;

$$F_N H^F_{i,N} + V_N + iH_{V,N+1} + L_{N-1}H^L_{i,N-1} - L_N H^L_{i,N} - M_N H^L_{i,N} - V_N H^V_{i,N} - U_N H^V_{i,N} - \quad Q_N = 0\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_(6)$$

Rearranging

$$F_N H^F_{i,N} + V_N + iH_{V,N+1} + L_{N-1} H^L_{i,N-1} - (L_N - M_N) H^L_{i,N} - (V_N - U_N) H^V_{i,N} - Q_N = 0 \qquad (7)$$

2.5. Column Dimension

2.5.1. Column Diameter (d)

The diameter of the column is calculated as follows;

$$d = \sqrt{\frac{4A_c}{\pi}} \qquad (8)$$

where; Ac is column cross sectional area; π is pi = constant; d is Column diameter

2.5.2. Column Cross-Sectional Area (A_c)

The cross sectional area is the space occupied by the column and is calculated as follows [15]);

$$Ac = \frac{Mr_i V_n}{0.88 \rho Va} \qquad (9)$$

where; A_c is cross sectional area of the column; V_n is Vapour flow rate of rectifying section; Va is actual vapour velocity Mr_1 is the molar weight of key component (most important); ρ is density of light key component.

2.5.3. Height of the Column

The height of the column is the distance from the bottom of the column to the top and is calculated as Sinnolt and Towler [15]

$$H_c = (N_a - 1) H_s + H \qquad (10)$$

where; H_c is actual column height; N_a is Actual number of plates; H_s is the Plate spacing; H is additional height required for column `operation or top and bottom dimension.

2.5.4. Downcomer Area

The space between the wall of the column and the tray is referred to as the downcomer. Downcomer is where the liquid falls from the top downwards to the bottom [15];

$$A_d = 0.12A_c \qquad (11)$$

where; A_d is downcomer area; A_c is cross-sectional area of the column

2.5.5. Wet Area

The wet area covers the area where the liquid in the plates fills the wet portion of the plate up to the weir length before entering the downcomer. The wet area is given by Sinnolt and Towler [15];

$$A_w = 0.88A_c \qquad (12)$$

where; A_w is Wet Area; A_c is Cross-sectional area of the column

2.5.6. Weir Length

The weir length is given by Sinnolt and Towler [15]:

$$L_w = 0.77d \qquad (13)$$

where; L_w is weir length; d is Diameter of column

2.5.6.1. Hole Area

Hole area A_h is the total area perforations on the tray and it is given by Sinnolt and Towler [15]:;

$$L_w = 0.77d \qquad (13)$$

where; A_h is Hole Area; A_c is Cross sectional area of the column

2.7. Operating Parameters

The feed properties and operating conditions of the crude distillation column obtained from literature [16] are given in Table 1

Table-1. Operating data of crude distillation unit

Bulk Properties			**Bottom stage pressure**	**225.5Kpa**	**32.70psia**
Standard Density	878.1kgm^3	29.32 API 60	Optional cond. Temp. Estimate	37.78°C	100.°F
Light Ends			Optional top stage temp. Estimate	121.1°C	250.0°F
Light Ends	Liquid Volume%		Optional bottom stage temp. Estimate	315.6°C	600.0°F
H_2O	0.0000		Flow Basic	Volume	
Methane	0.0225		**Side Options**		
Propane	0.3200		**Kerosene Side Stream**		
i-Butane	0.2400		Return stage	8 main Ts	
n-Butane	0.8200		Draw stage	9 main Ts	
Assay Input Table			Flow Basis	Stream ideal volume	
Assay Liquid Volume%	Boiling Temperature		Configuration	Steam stripped	
	°C	°F	Product Stream	Kerosene	
0.0000	-9.4444	15.00	Draw Specification	9 300barrel/day	
4.5000	32.248	90.00	**Diesel Side Stream**		
14.5000	115.648	240.00	Return stage	16 main Ts	

20.0000	154.568	310.00	Draw stage	17 main Ts
30.0000	224.068	435.00	Flow Basis	Standard ideal volume
40.0000	273.552	524.00	Configuration	Steam stripped
50.0000	326.928	620.00	Product Stream	Dieseel
60.0000	393.648	740.00	Draw Specification	1,925 barrel/day
70.0000	474.268	885.00	**Ago Side Stream**	
76.0000	520.972	969.00	Return stage	21 main Ts
80.0000	546.548	1015.00	Draw stage	22 main Ts
85.000	566.008	1050.00	Flow Basis	Stream ideal volume
Column Specifications			Configuration	Steam stripped
Number of stage (n)	29		Product Stream	AGO
Feed (ATMs) Stream	28 main Ts		Draw Specification	4500barrel/day
Inlet Stage	28 main Ts		**Steam Properties**	
Bottom Stage	Main steam		**Feed Steam**	
Condenser Energy stream	Q-condenser		Standard Ideal liquid Vol flow	662.4m^3/h
Condenser pressure	135.8Kpa	19.7 psia	Temperature	232.408°C
Condenser pressure Drop	62.05Kpa	9.000Psi	Pressure	517.1Kpa
Delta P	68.95Kpa		**For 2nd Active**	
Temperature	343.608°C		Specification value	-3. 5e7 Btu/hr
Main Steam			**Pump Around 3 (PA 3)**	
Mass flow	3402kg/hr		Return stage	21 main Ts
Temperature	375°F		Draw stage	22 main Ts
Pressure	1034Kpa		**For 1st Active**	
H_2O composition	1.000		Specification value	3e4 barrel/day
Diesel Steam			**For 2nd Active**	
Mass flow	1361kg/hr		Specification value	-3.5e7 Btu/day
Temperature	148.9°C		**Liquid Flow specification**	
Pressure	1034Kpa		Name	Over flash spec
H_2O composition	1.000		Stage	27 main Ts
Ago steam			Specification value	3500 barrel/day
Mass flow	2500lb/hr		**Duty Specification**	
Temperature	300°F		Name	KeroReboiler Duty
Pressure	50psia		Energy Stream,	Kero-ss-Energy
H_2O composition	1.000		Specification value	7.5e6 Btu/hr
			Vapour Flow Specification	
Pump Around			Name	Vapour
Pump Around 1 (PA 1)			Stage	Condenser
Return stage	1 main Ts		Flow Basis	Molar
Draw stage	2 main Ts		Specification value	0.000 barrel/day
For 1st Active			Reflux Ratio	1.000
Specification type	Flow rate		**Distillate Rate**	
Specification value	5e4 barrel/days		Reflux Ratio	1.000
For 2nd Active			Draw specification	Distillate Rate
Specification value	5. 5e7 Btu/hr		Name	Naphtha Product Rate
Pump Around 2 (PA2)			Draw	Naphtha@ColI
Return stage	16 main Ts		Specification value	2.3e4 barrel/day
Draw stage	17 main Ts		**Reflux Rate**	
For 1st Active			Liquid flow spec	Reflux Rate
Specification value	324 barrel/day		Vapour Product Flow	0.000 lbmol/hr

3. RESULTS AND DISCUSSION

Table 2a and 2b show the comparison between data obtained from literature Parthiban, et al. [16] and model prediction for a multi-component distillation of Bonny light crude, indicating that the model predictions compare reasonably well with the literature data; with a deviation ranging from 1.9 to 7.0 percent for the various components composition and 0.012 to 4.70 percent for the temperature variations respectively. The column dimension depicted in Table 2b shows a deviation ranging from 0 to 7.3 percent. A total of twenty-nine (29) trays were estimated, which is in agreement with literature data [16].

Table-2a. Comparison of Model Predictions with Literature Data

Components	Simulation Result		Literature Result		% Deviation	
	Composition	**Temperature**	**Composition**	**Temperature**	**Composition**	**Temperature**
Whole Naphtha	0.4506	41.81	0.4421	40.29	-1.923	-0.038
Straight Run kerosene(SRK)	0.1125	236.1	0.1210	248.0	7.025	4.798
Diesel Oil (D.O)	0.1783	253.0	0.1721	256.2	-3.603	0.012
Automotive Gas Oil (AGO)	0.0321	300.5	0.0330	312.2	2.727	0.038
Atmospheric Residue (A.R)	0.2265	355.0	0.2318	350.8	2.286	-1.675

Table-2b. Comparison of Simulation Result and Literature Result (Design Parameters)

Design Parameter	Simulation Result	Literature Result	% Deviation
Column Diameter(m)	1.558	1.531	-1.764
Area of Distillation Column(m^2)	1.907	1.892	-0.793
Height of Column (m)	17.048	17.060	0.070
Wet Area (m^2)	1.678	1.629	-3.008
Hole Area (m^2)	0.191	0.189	-1.058
Downcomer Area(m^2)	0.229	0.247	7.287
Weir length (m)	1.200	1.221	1.719
Tray Spacing (m)	0.500	0.500	0
Weir Height (m)	5.000e-002	5.00e-002	0
Tray Volume (m^3)	0884	0.824	-6.917

3.1. Sensitivity Analysis

A simulation model can be used to optimize plant performance by choosing the optimal set of operating condition such as flow rate, temperature, pressure, etc. In this work, the effect of temperature, pressure, flow rates, column properties were investigated.

3.1.1. Effect of Feed Flow Rate on Products Yield

The feed flow rate is the rate at which feed mixture (liquid, vapor or mixture of both) is pumped into the column. The flow of feed into a column can affect the quantity (moles/hr) and quality (concentration - mole fraction of the components/fractions).The effects of variation of the feed rate on the performance of the distillation column for the various components are shown in Table 3. The table shows that the higher the feed flow rate (increase in the feed rate) the greater the composition of the lighter ends in the bottom plate and the heavy components in the upper plate; the lower the feed rate (decrease in the feed rate) there is a reduction of the lighter ends in the bottom region and the heavier ends in the upper region. When the feed rate is increased, its velocity increases, its residence time (contact time of the vapor-liquid phases on each tray) in the column reduces, causing inefficient separation and a reduction in the percentage purity of each component, which might lead to weeping and decrease in the efficiency of the column performance.

Table-3. Effect of feed flow rate on products yield

Feed Flow Rate (Kgmole/hr)	**Component 1 Naphtha**	**Component 2 (S.R.K)**	**Component 3 (D.O)**	**Component 4 (A.G.O)**	**Component 5 (A.R)**
3119.63	0.421	0.109	0.172	0.032	0.267
2826.00	0.450	0.113	0.178	0.032	0.227
2544.00	0.485	0.117	0.184	0.032	0.183
2268.01	0.525	0.122	0.186	0.030	0.137

This inefficient separation could also be as a result of increased liquid or vapor flow rate as feed rates are increased. When the feed rate is decreased, its velocity decreases, its residence time in the column is increased, there is efficient separation and the percentage purity of each component is increased. However, decreases in the feed flow rates result in decreased vapor and liquid flow rates.

3.2. Effect of Temperature on Products Yield

The temperature distribution along the height of the column is depicted in Figure 4. The profile ranged from 41^{0}C (at the top) to 355^{0}C (at the bottom) and the temperature had a steady rise from the top (tray 1) through the stripping section.

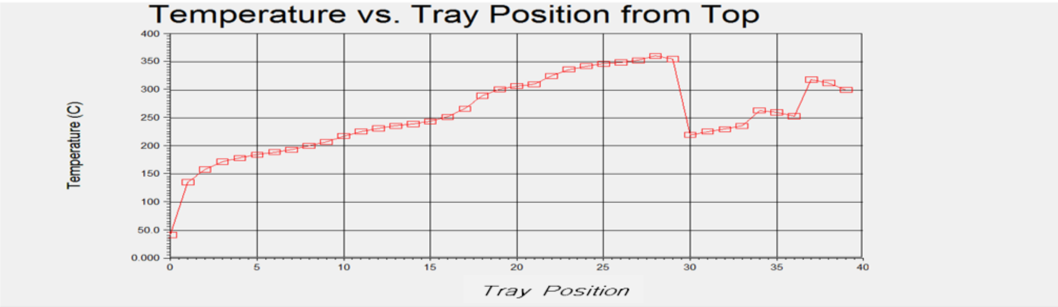

Figure-2. Effect of Temperature on the Products Yield

The effect of heat of reactions and the feed temperature input made the temperature curve to exhibit steady rise from top to bottom of column. It took a steep rise between tray 1 and 2, after which it maintained a steady increase in the stripping section to the bottom. The effect of bottom heat could have contributed to the high temperature profile in the stripping section. The column temperature is influenced by the heat of reactions and the fresh feed rates.. As the product (residue) leaves the column at the bottom, there is temperature drop, but as part of the bottom product (residue) are returned back into the column, the temperature rises as depicted in Figure 2. Immediately after tray 28 (which is the tray where the product leaves the column), the temperature begins to drop rapidly. The temperature later starts rising as a result of reboiling and refluxing the bottom product.. There is a steep drop in temperature after tray 29, because tray 29 is the last tray of the column and temperature decreases as the product leaves the column.

3.3. Effect of Pressure on Products Yield

Figure 3 shows the pressure distribution along the trays of the column. The pressure has steady rise from the top of the column downward. It took a steep rise between pressure of 135.8kpa and 198kpa, after which it maintained a steady rise down the bottom of the column

Pressure is controlled by refluxing in the column (i.e. as the residue is leaving the column, some amount of the residue is sent back into the column). As the residue leaves the column, there is pressure drop, which later rises as a result of the presence of the reboiler, which aid refluxing.

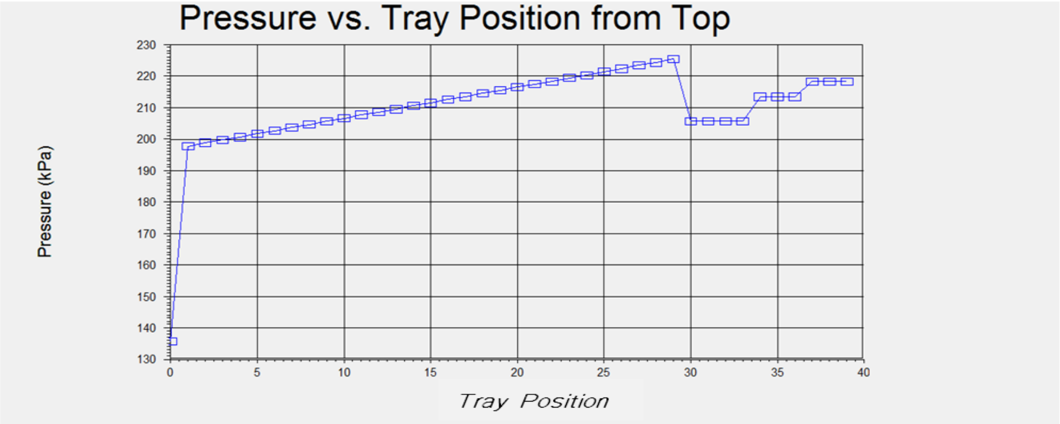

Figure-3. Effect of Pressure on the Products Yield

These explain why after tray 29 in Figure 3, (which is the last tray of the column and the point where the residue leaves the column), there is pressure drop which later increases due to refluxing in the column (bottom). There is steep drop in pressure after tray 29, because as the product leaves the column, pressure is expected to decrease progressively. The pressure rises steadily across the tray (from tray 1-29), because the difference in pressure between each tray is minimal (small).

3.4. Effect of Column Properties and Net Molar Flow on The Products Yield

The models were used to predict the column properties (density and molecular weight) and net molar flow of the five components of the crude oil mixture separated in a multicomponent distillation column. The effect of column column properties (density and molecular weight) and net molar flow of the five components; naphtha, straight run kerosene (SRK), diesel oil (DO), automotive gas oil (AGO) and atmospheric residue(AR) as predicted by the design equation from the process simulator (Aspen Hysys) on the twenty-nine (29) trays of the crude distillation unit obtained from literature [16] were shown in Figure 4 and 5 respectively.

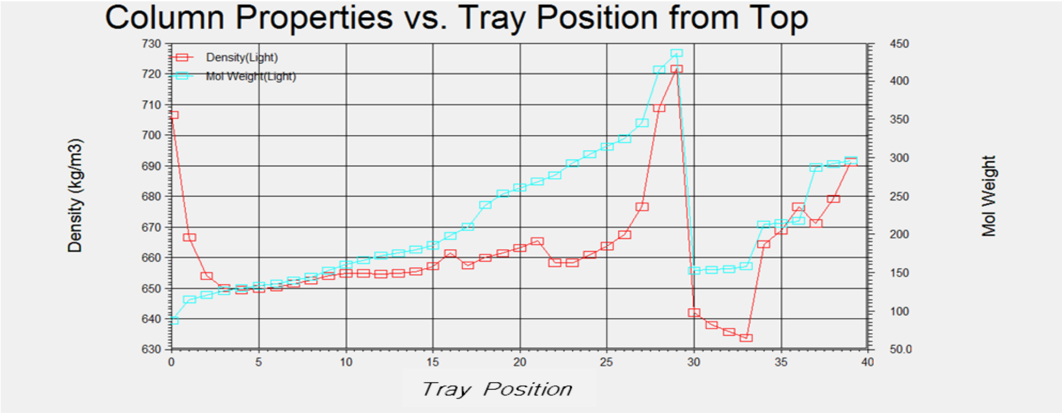

Figure-4. Effect of Column Properties on the trays

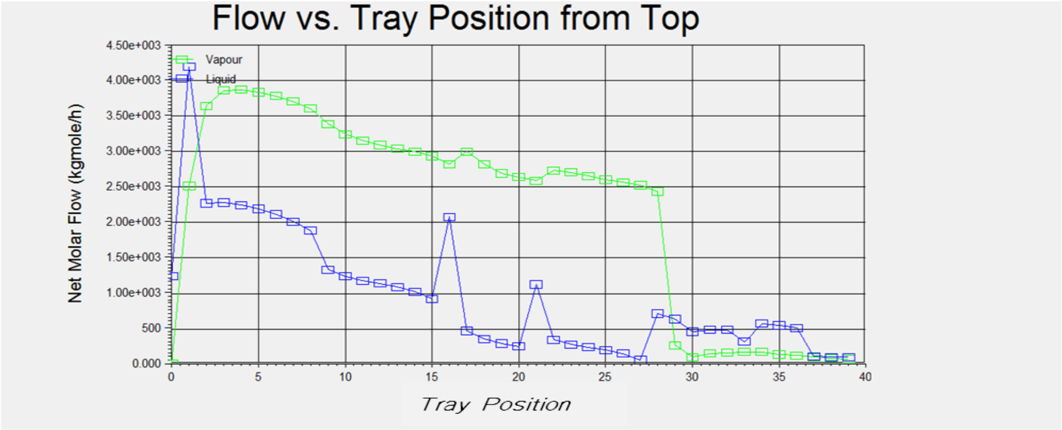

Figure-5. Effect of Net Molar Flow on the Products Yield

Figure 5 also shows the effect of eliminating pump-around PA1 on the vapour and liquid tray rates of the column. In the presence of the pump-around, liquid flow rates increase, as expected, to later decrease to a value in the first tray that is lower than the one observed without the pumparound in Figure 5. Vapour flow rates, decrease as expected. This contradicts column profiles presented by Watkins [17] where both liquid and vapour flow rates were reduced.

4. CONCLUSION

The design of the multi-component distillation column for processing of Bonny light crude is presented using advanced process simulation software (Aspen Hysys). The design parameters were column diameter, column cross sectional area, height of the column, downcomer area, hole area, weir length, wet area and tray spacing. The equations developed were capable of predicting compositions, partial pressures and temperature of the components from the mixtures of crude oil. The accuracy of the design parameters were validated with data obtained from literature for a functional industrial distillation unit. The simulation of the design models were performed using Aspen Hysys to obtain optimum values of the most significant variables/parameters (column diameters 1.558m, column height 17.048m, cross section area 1.907m^2, downcomer area 0.229m^2, tray spacing 0.5m, weir length 1.200m, hole area 0.191m^2 and wet area 1.678m^2). The result obtained from the steady state simulation shows that the feed flow rate, temperature and pressure influence the efficiency of the distillation column.

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