

Shortcut Modeling of an Existing Atmospheric Crude Distillation Column

Egamba, Kingsley C, Igbokwe Philomena K.

Department of Chemical Engineering, University of Uyo, Uyo, Nigeria

Department of Chemical Engineering, NnamdiAzikiwe University, Awka, Nigeria.

Abstract

A steady state shortcut model was developed for an existing atmospheric distillation column of a refinery in West Africa, which was validated using the plant operating data of the refinery. The model uses a new method to compute key component recoveries appropriate for the column product specifications, and also eliminates the need for stage by stage calculations in the stripping section of the column. The model is implemented by decomposing the atmospheric column into a sequence of thermally coupled simple columns with one net top product and one bottom product, and is capable of predicting flowrates and temperatures of products, column heat duties and true boiling point temperatures (TBP) of fractions. The average percentage deviations for product flowrates predicted by the model were 1.89%, 3.08%, 1.47%, 4.41%, and 9.98%, while the corresponding values for product temperatures were 2.34%, 2.16%, 0.91%, 3.28% and 3.42% respectively for residue, heavy gas oil, light gas oil, kerosene and naphtha. The developed shortcut model can be used to predict the outputs of the atmospheric column with good accuracy.

Keywords: Distillation Modeling, Shortcut Model, Atmospheric Column, Column Decomposition, Key Component Recoveries.

1. INTRODUCTION

Refinery crude oil processing is one of the largest applications of distillation as a separation technique in the chemical process industry. Existing refinery distillation units are highly energy intensive and have complex column configurations (Gadalla et al, 2003a). The operating conditions of an existing column affect the efficiency of the distillation occurring in the column and by extension the profitability of the process. The efficiency of an existing crude distillation unit (CDU) column can be improved by applying retrofitting schemes (Gadalla et al, (2003a); Gadalla et al, (2003b)), or by carrying out an operational optimization of the process variables. These procedures require suitable mathematical models relating the variables of the process.

Various rigorous and shortcut models have been proposed and applied to CDU operations. Rigorous models which are more accurate than the shortcut models, have significant convergence problems, and are more difficult to apply in simulation and optimization schemes. Shortcut methods on the other hand, are simple to calculate and robust in convergence (Gadalla et al, 2003b). The Fenske – Underwood – Gilliland (FUG) model is the most commonly applied shortcut model for multicomponent distillation. The modeling equations for the FUG model were originally derived for simple distillation columns employing reboilers, and hence require modifications for application in CDUs with complex column configurations and employing steam as the stripping agent.

Some researchers have extended the application of the shortcut modeling approach to atmospheric CDU

columns. Many of these models incorporate the Fenske and Underwood equations, and also apply stage by stage calculations in the stripping sections of the steam stripped CDU columns (Liu (2012); Chen (2008); Gadalla et al, (2003b); Suphanit (1999)). Application of the Underwood equations requires iterative procedures, which can result in convergence problems. The underwood equations can have multiple roots with the associated challenges, in cases where some distributed components have volatilities between those of the light and heavy key components. Also, applying stage by stage calculations in the stripping stages of the column makes the method semi-rigorous. The steady state shortcut modeling approach presented in this work does not employ the Underwood equations, and also does not require a stage by stage computation of the stripping stages, but combines overall column efficiency with an effective viscosity approach to account for the effect of stripping steam on the distillation process.

2. METHODOLOGY

The modeled column is the atmospheric distillation column of a refinery in West Africa, which is designed to process 125,000 bpd (830 m³/hr) of crude. The fractionator consists of 46 trays, and is equipped with 3 side strippers (each with 5 trays), 3 pump around circuits and a total condenser. The atmospheric column produces five product fractions, namely- distillate (mixture of naphtha and LPG), kerosene (KERO), light atmospheric gas oil (LAGO), heavy atmospheric gas oil (HAGO) and atmospheric residue (see Figure 1).

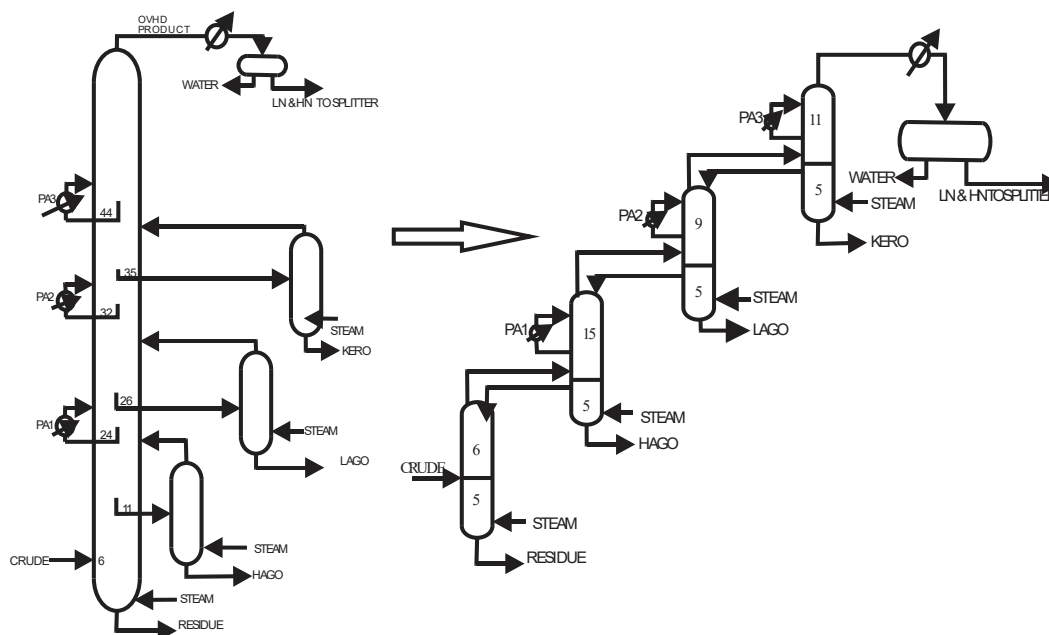


Figure 1: The decomposition of the existing column into a sequence of simple columns

The topped crude feed to the atmospheric column, was characterized and cut into 31 components, made up of a light end comprising; Methane; Propane; i-Butane; n-Butane; i-Pentane and n-Pentane, and 25 pseudocomponents. The Unisim R380 suite simulation package was employed for the characterization, using the

true boiling point (TBP) data of the crude, and selecting Peng Robinson equation as the fluid package, while the light end was auto calculated. The properties and compositions calculated by the simulator for the crude are presented in Table 1.

Table 1: Properties and Compositions of the components of the Characterized Crude

Compo	M.W	Tb (0K)	Tc (0K)	Pc (Bar)	ω	S.G (60/60)	WatsonK	μ 100 (cP)	Molfrac (Xfi)
methane	16.04	111.5	190.6	46.41	0.01150	0.300	19.2323	0.0122	0.0006
propane	44.10	230.9	369.8	42.57	0.15240	0.507	14.3899	0.0898	0.0032
i-butane	58.12	261.3	407.9	36.48	0.18480	0.564	13.7058	0.1563	0.0023
n-butane	58.12	272.5	425.0	37.97	0.20100	0.585	13.2905	0.1480	0.0035
i-pentane	72.15	300.9	460.2	33.34	0.22220	0.627	12.9585	0.1906	0.0014
n-pentane	72.15	309.1	469.5	33.75	0.25390	0.632	13.0570	0.2065	0.0008
hypo 1	74.43	320.8	495.4	36.35	0.22299	0.759	11.6948	0.3195	0.0182
hypo 2	78.43	335.5	511.4	35.14	0.25571	0.766	11.7620	0.3277	0.0162
hypo 3	85.59	350.4	528.6	34.14	0.28155	0.777	11.7504	0.3490	0.0356
hypo 4	95.17	365.7	546.7	33.06	0.30379	0.792	11.6983	0.4057	0.0666
hypo 5	103.65	380.4	563.0	31.56	0.32687	0.804	11.6834	0.4631	0.0666
hypo 6	110.64	392.6	576.3	30.33	0.34709	0.812	11.6798	0.5160	0.0830
hypo 7	117.85	408.1	592.4	28.69	0.37486	0.821	11.7033	0.5790	0.0529
hypo 8	125.70	420.5	605.6	27.63	0.39644	0.830	11.6909	0.6545	0.0574
hypo 9	133.48	435.5	620.8	26.23	0.42480	0.839	11.7092	0.7354	0.0550
hypo 10	142.62	450.3	635.7	25.02	0.45267	0.848	11.7108	0.8414	0.0641
hypo 11	152.98	464.6	650.3	23.98	0.47981	0.858	11.7001	0.9901	0.0620
hypo 12	162.59	478.3	663.8	22.99	0.50670	0.866	11.6995	1.1605	0.0474
hypo 13	173.72	493.5	678.6	21.94	0.53719	0.876	11.7000	1.3884	0.0539
hypo 14	186.55	507.2	692.3	21.15	0.56380	0.885	11.6791	1.7012	0.0659
hypo 15	196.44	520.9	705.1	20.24	0.59316	0.892	11.6915	1.9850	0.0471
hypo 16	209.11	536.0	719.3	19.33	0.62544	0.900	11.6944	2.4138	0.0120
hypo 17	222.82	550.2	732.8	18.57	0.65552	0.908	11.6875	2.9792	0.0084
hypo 18	237.00	564.6	746.3	17.82	0.68663	0.917	11.6834	3.7031	0.0103
hypo 19	252.11	578.8	759.5	17.13	0.71722	0.925	11.6755	4.6773	0.0158
hypo 20	264.04	589.9	769.8	16.60	0.74171	0.931	11.6715	5.6411	0.0192
hypo 21	274.48	604.4	782.2	15.80	0.77779	0.936	11.7009	6.6740	0.0580
hypo 22	283.79	622.5	796.8	14.76	0.82579	0.941	11.7580	7.7465	0.0269
hypo 23	296.23	637.6	809.8	14.05	0.86389	0.947	11.7770	9.6490	0.0190
hypo 24	310.34	650.6	821.4	13.56	0.89437	0.954	11.7717	12.4740	0.0147
hypo 25	329.72	664.3	834.2	13.15	0.92345	0.963	11.7403	17.9233	0.0120

The Fenske equation which was incorporated into the shortcut model being presented was derived for simple distillation columns having one top product and one bottom product. Hence to apply the Fenske equation, the column being modeled was decomposed into a sequence of partially thermally coupled columns, using the decomposition method of Liebmann cited in Chen (2008) and Liu (2012). The decomposition of the complex column is shown in Figure 1, while the resulting simple columns are depicted in Figure 2. The simple columns were then modeled sequentially to give the model of the fractionator.

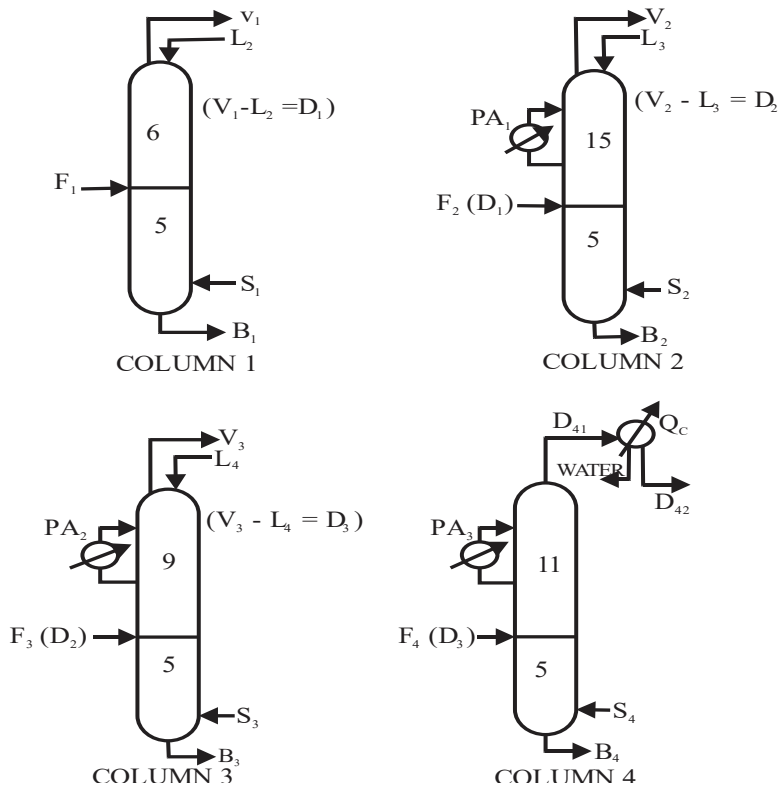


Figure 2: The simple columns showing the distribution of stages in each column section

The pairs of light key (LK) and Heavy key (HK) components used to model the separation occurring in each simple column were determined by a method described in Liu (2012), and is presented in Table 2. In specifying the separation occurring in the columns, the following simplifying assumptions were applied;

- i. The composition of the crude was assumed to be the same for the period covered by the plant operating data used.
- ii. Each pair of LK and HK was fixed for each simple column. Hence, the quality specification for each product

fraction of a simple column was fixed. The shortcut model calculates product flowrates and temperatures, column pump-around and condenser duties, as well as the T10 and T90 true boiling point temperatures (TBP) of HAGO, LAGO and KERO.

Table 2: Fixed Column and Operating Specifications for the Decomposed Simple Columns

Parameter	Column 1	Column 2	Column 3	Column 4
Rectifying Stages	6	15	9	11
Stripping Stages	5	5	5	5
LK Component	Hypo 14	Hypo 14	Hypo 9	Hypo 6
HK Component	Hypo 24	Hypo 24	Hypo 18	Hypo 8

3. MODEL DEVELOPMENT

The developed shortcut model combines the Fenske equation, material and energy balances in terms of the key component recoveries, a new method for computing key component recoveries, a modified overall column efficiency and energy balances to model the atmospheric column.

3.1 Material and Energy Balances:

In the decomposed scheme applied, vapour and liquid leave and enter a column respectively on the same stage. Hence, $(V_n - L_{n+1})$ can be taken as the effective distillate for column n. If the fractional recoveries of the key components in a column are defined by Equations 1 and 2, then material balances can be written for a simple column n as in Equations 3 to 5.

$$R_{LK,n} = \frac{Dx_{dLK,n}}{Fx_{fLK,n}} \quad 1$$

$$R_{HK,n} = \frac{Bx_{bHK,n}}{Fx_{fHK,n}} \quad 2$$

Total Material Balance:

3.2 Estimating relative volatilities of components:

The model computes relative volatilities from component K-values, using Equation 11.

$$\alpha_{i-r} = \frac{K_i}{K_r} \quad 11$$

Many authors have estimated K-values from correlations of the form of Equation 12 (Wilson (1968); Kumar et al, (2001); Almehaideb et al, (2002); Fattah (2012)).

$$K_i = \frac{P_{ci}}{P} \exp[(1 + \omega_i)f(T_{ri})] \quad 12$$

This shortcut model uses a modified form of the Wilson's correlation given in Equation (13) to compute component K-values.

$$K_i = \left(\frac{P_{ci}}{P}\right)^{0.745} \exp\left[5.37(1 + \omega^{0.714})\left(1 - \left(\frac{T_{ci}}{T}\right)^{0.755}\right)\right]$$

13

3.3 Computation of key component recoveries:

For each pair of selected LK and HK components in a simple column, a new method was used to compute the recoveries of these key components in terms of the minimum number of stages, using Equations 14 and 15.

3.4 Recovery of non-Key components:

Components lighter than the LK component and components heavier than the HK component were assumed not to be distributed (King, 1980). The recoveries of the components with volatilities between those of the LK and HK components were estimated from a form of the Fenske equation given in Equation 19.

$$D_{n-1} = D_n + B_n \quad 3$$

LK Component Material Balance:

$$D_{n-1}x_{dn-1,LKn}(R_{LK,n}) = D_n x_{dn,LKn} \quad 4$$

HK Component Material Balance:

$$D_{n-1}x_{dn-1,HKn}(R_{HK,n}) = B_n x_{bn,HKn} \quad 5$$

The energy balances (total stream) written for the simple columns are given in Equations 6 to 10.

$$F_1 h_{f1} + S_1 H_{S1} = D_1 h_{d1} + B_1 h_{b1} \quad \text{(column1) 6}$$

$$D_1 h_{d1} + S_2 H_{S2} = D_2 h_{d2} + B_2 h_{b2} + QPA_1 \quad \text{(column2) 7}$$

$$D_2 h_{d2} + S_3 H_{S3} = D_3 h_{d3} + B_3 h_{b3} + QPA_2 \quad \text{(column3) 8}$$

$$D_3 h_{d3} + S_4 H_{S4} = D_{41} h_{d41} + B_4 h_{b4} + QPA_3$$

$$D_{41} h_{d41} = D_{42} h_{d42} + Q_c \quad \text{(column4) 10}$$

The discussion on the derivation of these equations is published elsewhere (Igbokwe and Egemba, 2018).

$$R_{LK} = \frac{\alpha_{L-H}^{N_{min}(R)}(1 - \alpha_{L-H}^{N_{min}(S)})}{1 - (\alpha_{L-H}^{N_{min}(R)} \alpha_{L-H}^{N_{min}(S)})} \quad 14$$

$$R_{HK} = \frac{\alpha_{L-H}^{N_{min}(S)}(\alpha_{L-H}^{N_{min}(R)} - 1)}{(\alpha_{L-H}^{N_{min}(S)} \alpha_{L-H}^{N_{min}(R)}) - 1} \quad 15$$

Applying O'Connell's correlation for efficiency (Sinnott, 2005), with the average viscosity term replaced by an effective viscosity defined as in Equation 16, and setting the minimum number of stages in a column equal to 60% of the equilibrium number of stages (Smith (1963); Sinnott (2005)), gives the minimum number of stages for the rectifying and stripping sections as Equations 17 and 18.

$$\mu_{eff} = f(\mu_{av}, \mu_S) \quad 16$$

$$N_{min(R)} = (0.6) \left(\frac{51 - 32.5 \text{Log}(\mu_{eff} \alpha_{L-H})}{100}\right) (N_{ac(R)}) \quad 17$$

$$N_{min(S)} = (0.6) \left(\frac{51 - 32.5 \text{Log}(\mu_{eff} \alpha_{L-H})}{100}\right) (N_{ac(S)}) \quad 18$$

$$R_i = \frac{\left(\frac{1 - R_{HK}}{R_{HK}}\right) \alpha_{i-H}^{N_{min}}}{1 + \left(\frac{1 - R_{HK}}{R_{HK}}\right) \alpha_{i-H}^{N_{min}}} \quad 19$$

3.5 Computation of the enthalpy of streams:

The model computes the enthalpy of hydrocarbon streams from Equation 20.

$$H \left(\frac{\text{Kj}}{\text{kg}} \right) = H^{\text{ig}} - \frac{(2.326)RT_c}{M} \left[\frac{H^{\text{ig}} - H}{RT_c} \right] \quad 20$$

The first term on the right hand side of Equation (20) is the ideal gas enthalpy term which was computed using the Lee-Kesler method (Fahimet al, (2010); API (1997)), while the pressure effect (second term on the right) was computed using the Pitzer and Curl correlation (API,1997). The enthalpy of steam was computed from the correlation of Domijan and Kalpic (2005).

The viscosity and density of hydrocarbon components were determined from procedures

11A4.1 and 6A3.5 of API (1997) respectively. The model determines mixture properties using the mixing rule in Equation 21.

$$P_{\text{mix}} = \sum x_i P_i \quad 21$$

The model was validated by comparing model output with the operating data of the existing atmospheric distillation column.

4. RESULTS AND DISCUSSION

The flowrates and temperatures of product fractions predicted by the model were compared with plant values and presented in Tables 3 and 4 respectively. The column heat duties and the product TBPs computed by the model were not presented here because the plant operating data for these parameters were not available for comparison.

Table 3: Comparison of plant data and model predicted product flowrates

Test No	RESDF (m ³ /hr)			HAGOF (m ³ /hr)			LAGOF (m ³ /hr)			KEROF (m ³ /hr)			NAPHF (m ³ /hr)		
	PV	MV	%DV	PV	MV	%DV	PV	MV	%DV	PV	MV	%DV	PV	MV	%DV
1	151.1	153.3	1.46	26.5	26.6	0.53	124.9	121.8	2.48	91.0	87.0	4.40	86.6	77.8	10.16
2	152.3	153.4	0.72	25.7	26.6	3.50	123.9	122.0	1.53	91.0	87.1	4.29	86.7	77.8	10.27
3	154.2	153.7	0.32	26.0	26.6	2.27	125.0	121.9	2.48	91.0	87.0	4.40	83.4	77.7	6.83
4	143.7	154.2	7.31	25.7	26.6	3.70	120.7	122.2	1.24	95.0	87.3	8.11	91.4	78.1	14.55
5	152.3	154.0	1.12	27.2	26.7	1.80	123.1	122.4	0.57	91.0	87.6	3.74	87.6	78.3	10.62
6	155.7	155.2	0.32	28.0	26.9	3.83	124.8	123.2	1.28	91.0	87.9	3.41	86.8	78.6	9.45
7	151.8	154.8	1.98	26.8	26.9	0.56	125.0	123.1	1.52	91.0	87.9	3.41	86.9	78.5	9.67
8	151.6	153.9	1.52	27.9	26.7	4.13	125.0	122.2	2.24	91.0	87.3	4.07	85.8	78.0	9.09
9	158.0	153.4	2.91	27.4	26.6	2.74	122.9	122.1	0.65	91.0	87.2	4.18	87.4	77.5	11.33
10	154.3	156.3	1.30	25.4	27.4	7.75	125.0	125.9	0.72	91.0	89.7	1.43	86.2	79.4	7.89
Avg			1.89			3.08			1.47			4.14			9.98

PV: Plant value; MV: Model value; %DV: Percentage absolute deviation

Table 4: Comparison of plant data and model predicted product temperatures

Test No	RESDT (°C)			HAGOT (°C)			LAGOT (°C)			KEROT (°C)			NAPHT (°C)		
	PV	MV	%D V	PV	MV	%D V	PV	MV	%D V	PV	MV	%D V	PV	MV	%D V
1	338.	348.		334.	339.		284.	287.		192.	199.		136.	141.	
	6	1	2.81	6	9	1.58	9	7	0.98	0	2	3.75	7	4	3.44
2	339.	348.		333.	341.		284.	288.		192.	200.		136.	141.	
	4	4	2.65	6	2	2.28	0	5	1.58	4	0	3.95	5	6	3.74
3	339.	347.		332.	339.		285.	286.		192.	197.		134.	139.	
	3	8	2.51	9	2	1.89	9	8	0.31	1	2	2.65	8	2	3.26
4	338.	344.		328.	334.		287.	283.		192.	194.		133.	137.	
	6	7	1.80	3	2	1.80	5	7	1.32	1	5	1.25	7	1	2.54
5	338.	347.		334.	339.		285.	287.		193.	200.		137.	142.	
	5	8	2.75	0	9	1.77	1	9	0.98	5	1	3.41	1	0	3.57
6	340.	348.		333.	340.		285.	287.		192.	198.		135.	139.	
	1	0	2.32	2	0	2.04	6	2	0.56	6	2	2.91	3	9	3.40
7	339.	348.		333.	341.		287.	288.		193.	199.		136.	141.	
	8	5	2.56	5	0	2.25	0	6	0.56	1	9	3.52	3	2	3.60
8	339.	347.		332.	339.		286.	287.		192.	198.		135.	140.	
	8	9	2.38	4	4	2.11	8	2	0.14	6	4	3.01	6	7	3.76
9	339.	347.		332.	339.		287.	288.		193.	199.		134.	138.	
	9	0	2.09	4	7	2.20	4	0	0.21	0	0	3.11	0	3	3.21
10	339.	345.		332.	345.		286.	293.		193.	203.		134.	139.	
	9	0	1.50	8	0	3.67	4	3	2.41	8	9	5.21	8	7	3.64
Avg			2.34			2.16			0.91			3.28			3.42

PV: Plant value; MV: Model value; %DV: Percentage absolute deviation

The absolute deviations of the predicted flowrates for residue, heavy atmospheric gas oil, light atmospheric gas oil and kerosene were all below 10%, while the maximum percentage deviation for naphtha was 14.55%. The average percentage deviations were 1.89%, 3.08%, 1.47%, 4.14% and 9.98% for residue, heavy atmospheric gas oil, light atmospheric gas oil, kerosene and naphtha flowrates respectively. The product fractions temperatures predicted by the model had maximum percentage deviations of 2.81%, 3.67%, 2.41%, 5.21%, and 3.76% for residue, heavy atmospheric gas oil, light atmospheric gas oil, kerosene and naphtha respectively, while the corresponding average values were 2.34%, 2.16%, 0.91%, 3.28%, and 3.42%. The absolute deviations for the predicted temperatures were also generally below 10°C. A percentage deviation of 10% or less is considered acceptable. The low values of the deviations observed for the model outputs is an indication that the model can be used to predict product flowrates and temperatures in an existing atmospheric crude distillation column of a refinery.

5.0 CONCLUSION

A shortcut model of an existing refinery atmospheric crude distillation column has been developed. A new method for determining key component recoveries, which was incorporated into the model, was able to transform industry specifications into appropriate key component and their recoveries required for the implementation of the model on the column. The model does not require initial guesses to compute component recoveries, nor require stage by stage calculations in the stripping section of the atmospheric column. The average percentage deviations predicted by the model for product flowrates and temperatures when compared with plant values were below 10%. The deviations for temperatures were also generally below 10°C. Hence the developed shortcut model can be used to predict the product flowrates and temperatures of the existing CDU column with sufficient accuracy. A MATLAB code was written to execute the shortcut model on the existing refinery atmospheric column.

Notations

h	Enthalpy of liquid
H	Enthalpy of vapour
HK	Heavy key component
LK	Light key component
N_{ac}	Actual number of stages in a column
$N_{min(i)}$	Minimum number of stages in section i of a column
P_c	Critical pressure
P	Total pressure
QC	Condenser duty

QPA _i	Heat duty of pump around i
R_i	Recovery of component i
T	Temperature of stream
T_c	Critical temperature
T_r	Reduced temperature
x_{bi}	Mole fraction of component i in bottom product
x_{di}	Mole fraction of component i in top product
x_{fi}	Mole fraction of component i in feed
ω	Accentric factor

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