Multicomponent Distillation Column Profile based on iterative convergence method.

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Abstract: Determination of column stage profile is crucial in the design of distillation column. Process industries are going digital and require simulation packages inbuilt for their own design. Simulators today, however, are in closed system and are not customizable with the digital applications. A fundamental algorithm provided then transcribed to the required system may solve the purpose and thus process design as per individual industrial requirements is possible. This project aims to build algorithms to generate a multicomponent distillation tray profile. Microsoft VBA platform is used to test these algorithms and generate such profiles. The Peng-Robinson equation of state is used for generating VLE Data. The project develops its own mathematical method to compute the stage balance. A Pentane-Hexane-Heptane separation scenario is taken for case study in this project and its profile is generated for analysis.

Index Terms – **Column Profile, Vapor-Liquid Equilibrium (VLE), Activity Coefficients, PR Equation of state.**

I. INTRODUCTION

The chemical industry performs conversion processes, and separation operations to produce chemicals. Distillation is the most popular separation operation where components in a mixture are separated based on their property of relative volatility. It is a stage separation process by vapor, and liquid contact where vapor goes on rectifying high volatile components as it moves from bottom to top stages. On the contrary, the liquid gets stripped out of high volatile components as it moves from top to bottom.

Thus, the stage equilibrium is a critical component of distillation tower design, and proper hydraulic engineering must be performed before design or operation. A tray profile thus generated through various simulation software like Aspen-Tech or ChemCAD provides the firsthand calculation basis. However, their computation methods are in the black box and thus cannot find application in custom required software for industries. Also, the process industries are moving towards digitalization and these computation methods are required to build up an accurate design model.

This project aims to provide a similar solution of tray profiles. However, this project does not guarantee the exact data congruence with actual operation. The convergence of this software is concerned only with the laws of stoichiometry and thermodynamics. The Peng-Robinson equation of state is employed for generation of the Vapor-Liquid Equilibrium data.

The chemical properties are available in open source such as Yaw's Chemical Properties Handbook (1) or the Perry's Handbook (2). A set of saturated hydrocarbon databanks is made using these sources. To computation, we use the Microsoft Office VBA platform. VBA Excel is ideal for coding iterative calculations and producing data in spreadsheets. VBA being an application language provides the comfort of fewer syntaxes.

We consider a separation process of Pentane with 99% recovery from a mixture of Pentane-Hexane-Heptane system. We analyze the results for feasibility, thermodynamic and stoichiometric convergence for the tray profile.

II. MATHEMATICAL MODELING OF MULTI-COMPONENT STAGES.

Multi-component distillation column stage profiles can be estimated by conducting rigorous component, mass, and energy balance through all the stages. For each stage being at its thermodynamic equilibrium, the principle of vapor-liquid equilibrium is followed. For stage N, the liquid stream entering from the top stage is noted as LN-1, and the vapor stream entering from the next stage is noted as VN+1. Their temperature, pressure, and composition are respective to their source stages. The vapor stream exiting the stage is noted as VN, and the Liquid stream exiting the stage is noted as LN. VN and LN are in vapor-liquid equilibrium (VLE). In other words, the component composition of the VN, and LN are such that the vapor dew point and liquid bubble point are equal.
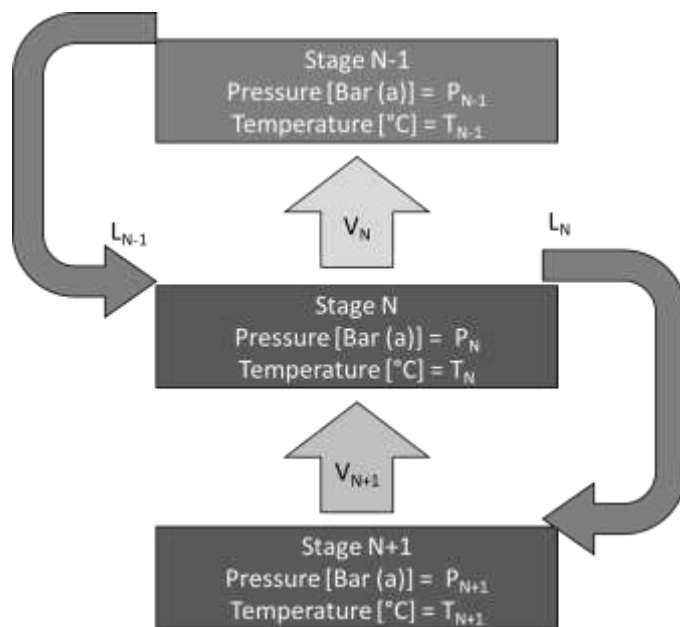
Figure 1 Typical Distillation Column Stage

Peng Robinson Equation of State

Thus, for a component i of the mixture at VLE (3).

$$y_i = K_i * x_i$$

(1)

where y denotes the vapor molar composition, x denotes the liquid molar composition, and K is their equilibrium constant specific to the component. This equilibrium constant gets derived from various thermodynamic equation of state depending on the type of system, and its operating parameters. For this study, we have considered the Peng-Robinson equation of state (2-4).

$$P = \frac{RT}{V - b} - \frac{a(T)}{V(V + b) + b(V - b)}$$

(2)

$$a(T) = \propto a(T_c)$$

(3)

$$a(T_c) = 0.45724 \frac{\propto R^2 T_c^2}{P_c}$$

(4)

$$b = 0.07780 \frac{RT_c}{P_c}$$

(5)

$$\propto = \left(1 + \kappa\left(1 - \sqrt{\left(\frac{T}{T_c}\right)}\right)^2\right)$$

(6)

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

(7)

where,
P is Pressure (Pa)
V is Molar Volume (m3 mol-1)
R is the gas constant (8.314 J mol-1 K-1)
T is Absolute Temperature (K)
P_c is the critical pressure for the component of interest (Pa)
T_c is the critical temperature for the component of interest (k)
ω is the accentric factor for the component of interest.

The PR Model for mixing

$$a = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij}$$

(8)

$$b = \sum_{i=1}^{n} x_i b_i$$

(9)

$$a_{ij} = (1 - k_{ij})(a_i a_j)^{\frac{1}{2}}$$

(10)

where,

a is the PR attraction parameter.

a_i is the pr attraction parameter for component i.

b   is the PR co-volume for the mixture.

b_i is the PR covolume for the component i.

k_{ij} is the PR binary interaction parameter.

We note here that the parameter kij is evaluated from other models. Nishium (4-7) suggest the following model for hydro-Carbon interaction.

$$a_{ij} = m_{ij}\sqrt{a_i a_j}$$

(11)

$$m_{ij} = C + D * \left(\frac{V_{ci}}{V_{cj}}\right) + E * \left(\frac{V_{ci}}{V_{cj}}\right)^2$$

(12)

$$C = c_1 + c_2 * |w_i + w_j|$$

(13)

$$D = d_1 + d_2 * |w_i + w_j|$$

(14)

$$C_1 = 1.041 \; ; C_2 = 0.11$$

(15)

$$d_1 = -0.0403; \; d_2 = 0.0367; E = 0$$

(16)

Thus, the PR equation of state, and mixing rules is particular about the critical parameters of the individual chemical. For the case scenario for this project, we consider a databank of chemicals referred from Yaw's Chemical Properties Handbook (1).

Sr.No.	Compound	Tc (K)	Pc (MPa)	w	Zc	Vm (cm3/mol)	k	b	Mol. Wt (g/mol)
1	Methane	190.6	4.604	0.011	0.288	99.13	0.3916	26.78	16.04
2	Ethane	305.4	4.88	0.099	0.284	147.77	0.5247	40.48	30.07
3	Propane	369.8	4.249	0.152	0.281	203.33	0.6028	56.29	44.09
4	n-Butane	425.2	3.797	0.193	0.274	255.10	0.6622	72.43	58.12
5	Isobutane	408.1	3.648	0.177	0.282	262.28	0.6392	72.36	58.12
6	n-Pentane	469.7	3.369	0.249	0.269	311.80	0.7419	90.18	72.15
7	Isopentane	460.4	3.381	0.228	0.27	305.68	0.7122	88.08	72.15
8	Neopentane	433.8	3.199	0.196	0.269	303.28	0.6666	87.71	72.15
9	n-Hexane	507.4	3.012	0.305	0.264	369.75	0.8199	108.96	86.17
10	n-Heptane	540.3	2.736	0.349	0.263	431.80	0.8800	127.73	100.2
11	n-Octane	568.8	2.486	0.396	0.259	492.68	0.9430	148.00	114.22
12	n-Nonane	595.7	2.306	0.437	0.255	547.67	0.9971	167.09	128.25
13	n-Decane	618.5	2.123	0.484	0.249	603.11	1.0579	188.44	142.28
14	n-Dodecane	658.2	1.824	0.575	0.238	714.04	1.1722	233.41	170.33
15	n-Tetradecane	696.9	1.438	0.57	0.203	817.93	1.1660	313.47	198.38
16	n-Hexadecane	720.6	1.419	0.747	0.22	928.85	1.3761	328.47	226.43

Table 1 Components and their properties

The model predicts the Vapor-Liquid Equilibrium based on the fugacity coefficients as

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0$$

(17)

$$A = \frac{aP}{R^2 T^2}$$

(18)

$$B = \frac{bP}{RT}$$

(19)

$$Z = \frac{PV}{RT}$$

(20)

Being a cubic equation, the solution of 'PR Polynomial form' leads to 3 roots. The imaginary roots have no significant meaning. In the case of a single or equal root, a single phase of the chemical or chemical mixture will exist. In the case of three unequal roots, one root will have no physical meaning, and the other roots will have the compressibility factor of liquid, and vapor.

Based on the compressibility factor, the fugacity coefficients of the state are evaluated as

$$ ln\phi_k = \frac{b_k}{b}(1 - Z) - \ln(Z - B) - \frac{A}{2\sqrt{2}}\left(\frac{(2\sum_{i=1}^{n} x_i a_{ik})}{a} - \frac{b_k}{b}\right)\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) $$

(21)

where ϕ is the fugacity coefficient for component k.

Thus, the vapor-liquid equilibrium equation thus derived as given below.

$$ y_i = \frac{\phi_i^L}{\phi_i^V} x_i \ Or \ y_i = k_i x_i $$
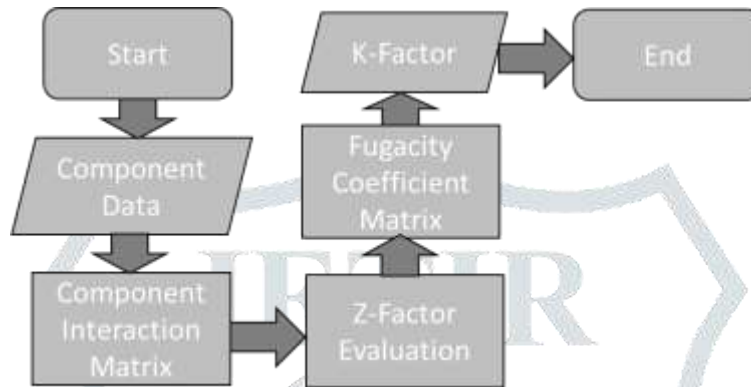
(22)

Figure 2 PR K Factor Evaluation Algorithm

Bubble Point and Dew Point

The bubble point and dew point are computed as:

  Bubble Point

  The Temperature which satisfies the given equation

  $\sum (x_i * K_i) = 1$ Where x_i is mole fraction of liquid component i and k_i = f(x_i , Pressure) from Peng Robinson Method.

  Dew Point

   The Temperature which satisfies the given equation

  $\sum (y_i / K_i) = 1$ Where y_i is mole fraction of vapor component i and k_i = f(y_i , Pressure) from Peng Robinson Method.

Stage Balance

For a conservative distillation column operation, the process feed, Distillate purity, and Bottom compositions are well-defined based on which the column is sized. The degree of separation is determined by the amount of energy supplied to the reboiler. Based on the mentioned conditions, the operating pressure and temperature of the column get fixed.
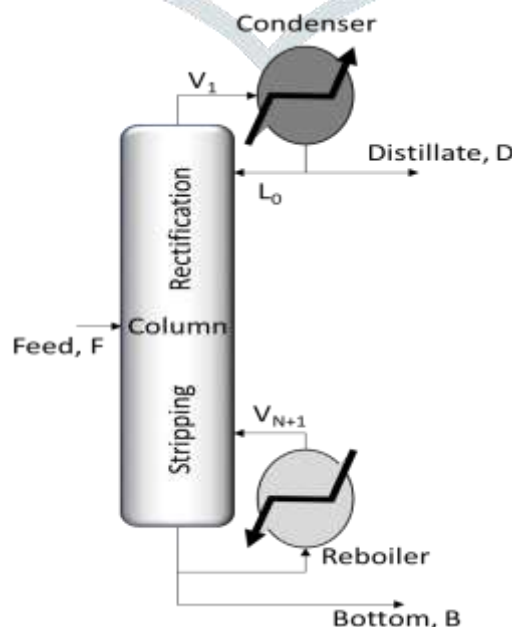

Figure 3 Typical Distillation Column

For discussion, an N tray column is illustrated with tray count starting from top to bottom. Subscripts are used to demonstrate the source stage of the stream flow. For a reflux ratio R, and Distillate flow D,

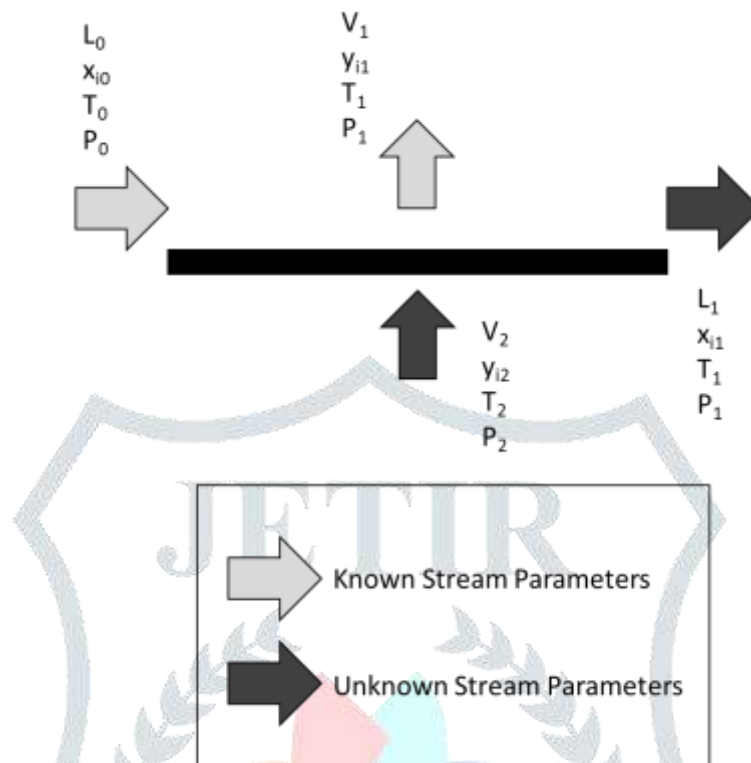$$R = \frac{L_0}{D}$$

(23)

$$V_1 = L_0 + D$$

(24)

Figure 4 Distillation Stage Balance

Since, V1, and L1 are in equilibrium,

$$y_{i1} = K_{i1} * x_{i1}$$

(25)

For Multi-component mixtures as given by Bhatt (2009) (4)
1. Vapor Composition based on Liquid composition.

$$y_i = \frac{k_i * x_i}{\sum k_i * x_i}$$

(26)

2. Liquid Composition based on Vapor Composition

$$x_i = \frac{\frac{y_i}{k_i}}{\sum \frac{y_i}{k_i}}$$

(27)

The molar composition x of liquid stream are evaluated. For conducting Mass, energy, and component balance, we write In, and Out streams in a 2 X 2 Matrix.

Flow In	Flow Out
V2	V1
L0	L1

For Flow In = Flow Out
1. Mass Balance

$$V_2 - L_1 = V_1 - L_0$$

(28)

2. Energy Balance

$$(\lambda_2 + C_{p2} * T_2) * V_2 - C_{p1} * T_1 * L_1 = (\lambda_1 + C_{p1} * T_1) * V_1 - C_{p0} * T_0 * L_0$$

3. Component Balance

$$y_{2i} * V_{2i} - x_{1i}L_{1i} = y_{1i}V_{1i} - x_{0i}L_{oi}$$

Thus, we get three equations, and three unknown systems. However, the properties of specific heat and latent heat are dependent on the composition. Thus, this leads to a cyclic iterative calculation. With iterative calculations enabled spreadsheet or code-based spreadsheet, one can compute this system as given in the algorithm below.

Now, V2, and L1 computed, one can follow the thread (V3,L2)- (V4,L3)- (V5,L4)- (V6,L5)……- (VN+1,LN)

The profile convergence is evaluated by the energy of VN+1 in congruence with the energy of liquid going to the reboiler plus reboiler duty. In case of a mismatch, the overall mass and energy balance of the column is, and the reflux ratio is improvised by iterations. With the improvised reflux ratio, the system will converge.

The feed tray has an additional liquid or vapor stream getting added to the flow, with the streams modified, the same balance method will be followed.

By conducting rigorous calculations, the stage compositions, pressure, and temperature matrix is the solution. With standard thermodynamic equations of properties, one can compute the phase density, viscosity, and surface tension required for tray hydraulics.
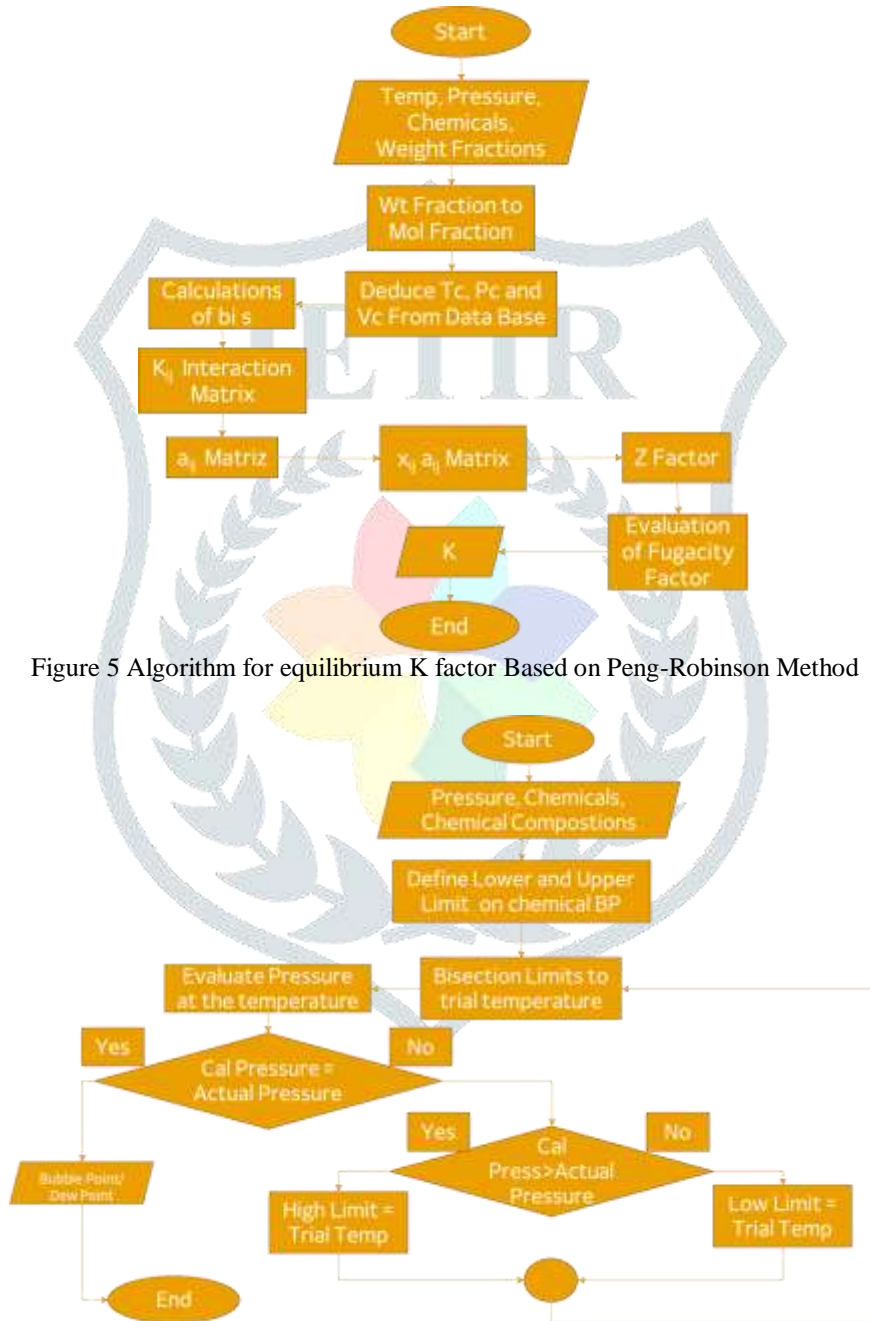
III. ALGORITHMS

Figure 5 Algorithm for equilibrium K factor Based on Peng-Robinson Method

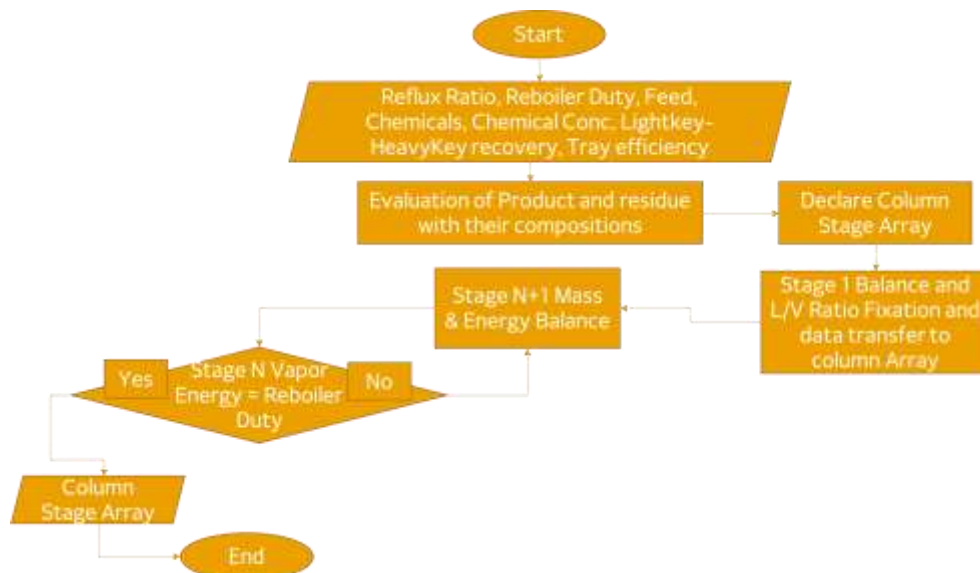Figure 6 Algorithm for Dew point and Bubble Point
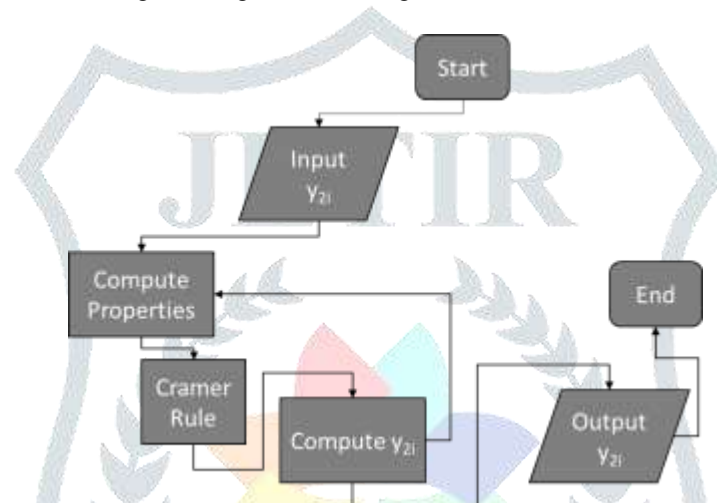
Figure 7 Algorithm for Stagewise Column Balance

Figure 8 Stage Balance Algorithm

IV. RESULTS AND DISCUSSION

An appropriate code is constructed in VBA Excel. We create level 1 User Defined Function (UDF) which take concentration of components and operating temperature to give output of basic properties like density, vapor pressure, etc. Level 2 functions are those which use the level 1 properties and perform iterative calculations. These are functions such as saturation point temperature, VLE vapor to liquid or vice-versa liquid to vapor, Cramer's rule and so. We then construct level 3 function which does the stage balance based on iterations. These functions are intermingled, and only level 3 functions are called upon on the spreadsheet. Since stage balance is a multi-output function, we store the outputs of one process in arrays. Even the inputs are stored in the same array since the characteristic of the output is linked to the set of inputs. Now mathematically, for a many-one functions, the specific set of inputs have specific output. Thus, if this level 3 function is called in the spreadsheet, first the program inspects the inputs stored in the array. For the same inputs, the same output matrix is produced. The outputs thus have been assigned with a particular index number related to the matrix. For instance, index 1 will give output of stage pressure, index 2 gives output of stage temperature and so on.

To initiate the calculation, we put the respective flow streams with known values at their respective spreadsheet addresses. We add the inputs to the UDF give indexes as per the spreadsheet address. Now for the current system, a specific stage pressure drop is selected as 0.01 bara. With all inputs at place, the UDF set is copied to the next row. Each row represents a stage of operation. For 30 stages with condenser and reboiler included, we generate a total of 28 tray profile as shown in the table.

There are certain key points of observation. We check the mass and energy balance of stages which we found was perfectly matching. Next, we observe the increase in purity of low volatile components as we move towards the top trays. Also, the increase in the high volatile component at the bottom is observed. Since the column is based upon stripping out pentane, we observe a smooth profile of pentane distribution compared to distribution hexane and heptane. The feed tray being the 13 trays, a sudden increase in liquid load is observed and still the equilibrium of energy and mass balance is maintained. This can be related with simulator results as well. There are no outlier points observed in the data thus generated. As far as the profile is concerned, the desired profile is thus obtained for the given scenario.

Tray Parameters			Vapor Conc [w/w]				Liquid Conc [w/w]			
Tray	Temp [Deg C]	Pressure [Bar a]	Vapor Load [kg/h]	Pentane	Hexane	Heptane	Liquid Load [kg/h]	Pentane	Hexane	Heptane
0	38.8	1.1					6564.53	99.00%	1.00%	0.00%
1	39.14	1.1	9582.73	99.00%	1.00%	0.00%	6539.57	97.07%	2.93%	0.00%
2	40.06	1.11	9557.77	97.68%	2.32%	0.00%	6515.95	93.40%	6.60%	0.00%
3	41.54	1.12	9534.15	95.18%	4.82%	0.00%	6481.88	87.00%	13.00%	0.00%
4	43.81	1.13	9500.08	90.81%	9.19%	0.00%	6445.78	77.25%	22.75%	0.00%
5	46.91	1.14	9463.98	84.18%	15.81%	0.00%	6426.14	65.02%	34.96%	0.02%
6	50.44	1.15	9444.34	75.88%	24.11%	0.01%	6434.02	52.81%	47.13%	0.06%
7	53.73	1.16	9452.22	67.56%	32.40%	0.04%	6461.17	42.95%	56.84%	0.21%
8	56.35	1.17	9479.37	60.79%	39.06%	0.14%	6487.91	36.14%	63.23%	0.63%
9	58.31	1.18	9506.11	56.10%	43.47%	0.43%	6497.67	31.81%	66.45%	1.75%
10	59.98	1.19	9515.87	53.12%	45.69%	1.19%	6475.74	28.91%	66.49%	4.60%
11	61.99	1.2	9493.94	51.19%	45.67%	3.14%	6407.57	26.40%	62.35%	11.25%
12	65.17	1.21	9425.77	49.65%	42.70%	7.65%	6300.85	23.36%	52.40%	24.24%
13	70.14	1.22	9319.06	47.86%	35.75%	16.39%	20849.88	19.59%	37.29%	43.12%
14	71.06	1.23	8868.08	45.91%	37.27%	16.82%	20934.26	18.54%	38.19%	43.27%
15	72.21	1.24	8952.45	43.22%	39.38%	17.40%	21042.80	17.13%	39.40%	43.47%
16	73.63	1.25	9061.00	39.66%	42.17%	18.17%	21180.73	15.35%	40.94%	43.71%
17	75.32	1.25	9198.93	35.22%	45.66%	19.12%	21350.05	13.25%	42.75%	43.99%
18	77.19	1.26	9368.25	30.08%	49.72%	20.20%	21546.95	10.97%	44.74%	44.29%
19	79.12	1.27	9565.15	24.59%	54.06%	21.35%	21760.45	8.69%	46.74%	44.56%
20	80.98	1.28	9778.64	19.22%	58.31%	22.47%	21974.51	6.60%	48.59%	44.80%
21	82.66	1.29	9992.71	14.40%	62.12%	23.47%	22173.58	4.83%	50.17%	45.00%
22	84.07	1.3	10191.78	10.39%	65.30%	24.31%	22346.90	3.42%	51.43%	45.15%
23	85.23	1.31	10365.10	7.26%	67.76%	24.99%	22490.48	2.36%	52.36%	45.29%
24	86.17	1.32	10508.68	4.93%	69.52%	25.55%	22605.85	1.58%	52.96%	45.46%
25	86.97	1.33	10624.05	3.26%	70.62%	26.13%	22697.59	1.04%	53.18%	45.78%
26	87.75	1.34	10715.78	2.09%	70.94%	26.98%	22771.73	0.66%	52.80%	46.54%
27	88.75	1.35	10789.93	1.28%	70.00%	28.72%	22836.90	0.40%	51.15%	48.45%
28	90.45	1.36	10855.10	0.73%	66.44%	32.83%	22916.09	0.22%	46.79%	52.99%
0	93.76	1.37	10934.28	0.35%	57.19%	42.46%				

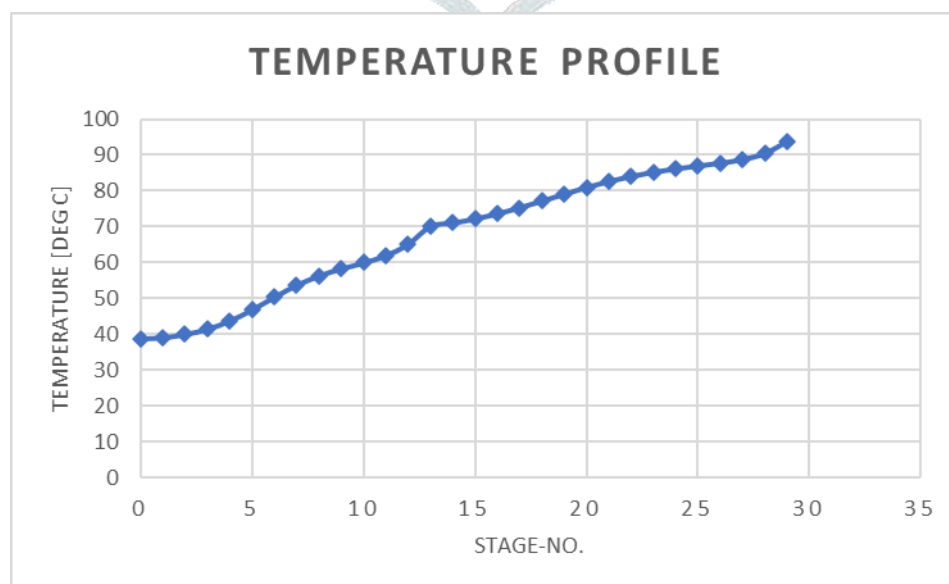Table 2 Column Tray Profile

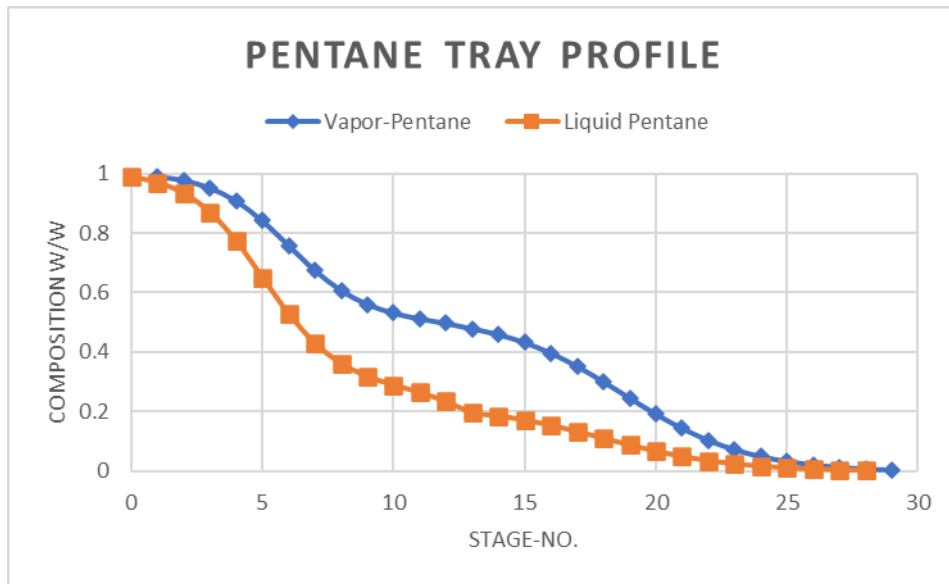Figure 9 Temperature Profile of Column
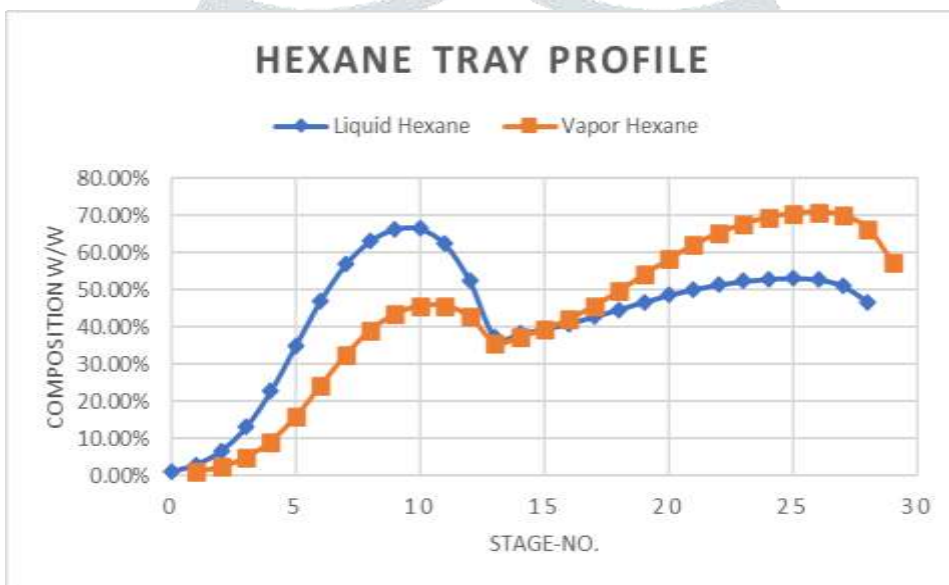
Figure 10 Pentane Component Tray Profile
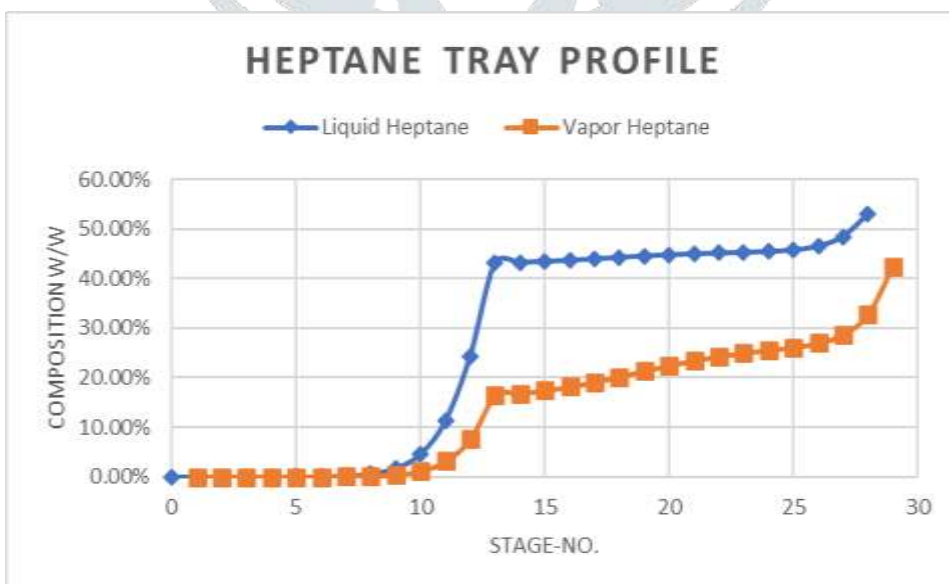

Figure 11 Hexane Component Tray Profile

Figure 12 Heptane Component Tray Profile

V. CONCLUSION.

The algorithms generate the tray profile successfully and can be used for detail distillation column design. However, this project does not guarantee the congruence of results with the actual operating conditions. These algorithms provide a fair approximate data for performing design calculations. Thus, this methodology is suitable for conservative design and simulation. Also, for case of optimization, the same algorithms can be utilized. This effort will suitably contribute to the industry's digital initiative of engineering design.

VI. ACKNOWLEDGMENT

VII. ABBREVIATIONS

A	the PR attraction parameter.
a_i	the PR attraction parameter for component i.
B	the PR co-volume for the mixture.
b_i	the PR co-volume for the component i.
B	Column Bottom flow [kg hr^{-1}]
Cp	Specific Heat [kCal kg^{-1} K^{-1}]
D	Column Distillate [kg hr^{-1}]
K	Vapor-Liquid-Equilibrium Constant
k_{ij}	the PR binary interaction parameter.
L	Reflux [kg hr^{-1}]
P	Pressure [Pa]
P_c	the critical pressure for the component of interest [Pa]
R	the gas constant [8.314 J mol^{-1} K^{-1}]
T	Absolute Temperature [K]
T_c	the critical temperature for the component of interest [k]
x	Liquid Component composition [mol/mol]
y	Vapor Component composition [mol/mol]

Greek Symbols

ρ_L	Liquid Density, [Kg m^{-3}],
ρ_v	Pv Vapor Density, [Kg m^{-3}],
λ	Latent Energy [kCal kg^{-1}]
ω	the accentric factor for the component of interest.

Subscripts

i	ith component
j	jth component
c	Critical Parameter
N	Nth Stage

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