



Vapor-Liquid Equilibrium Calculation of Multi-Components System with Estimation of Pre-Heat Temperature

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Authors' contributions

This work was carried out in collaboration between all authors. Author FOC designed the study and wrote the protocol. Author OTO performed the statistical analysis and wrote the first draft of the manuscript. Authors FOC and BOE managed the analyses of the study. Author OTO managed the literature searches. All authors read and approved the final manuscript.

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ABSTRACT

This general process design for multi-components vapor-liquid equilibrium flash calculation of a two-phase system comprises bubble and dew point calculations, estimation of the flash point, calculations of the vapor split and resulted compositions with flow rates in each of the liquid and vapor phases and estimation of the pre-heat temperature needed for a specific vapor split via unprecedented theories. The technique employed entails prediction of the equilibrium temperature, based on the critical temperatures of the feed's components, which in turn is used to estimate the corresponding flash pressure. The theories entail accommodate any light hydrocarbons' mixture and other molecules which are of relatively uncomplicated molecular force fields, as in the case of natural gas liquid. Appropriate gases and liquid properties correlations parameters were obtained from the literatures and used in different equations most suitable for vapor-liquid equilibrium calculations of any light hydrocarbons' mixture and other mixtures of relatively uncomplicated molecular force fields. The computer implementation puts forward for this design calculation, which can handle up to twelve components, aids the calculations of vapor-split, which requires several iterations, and other results.

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1. INTRODUCTION

Vapor-liquid equilibrium (VLE) is a state or condition where the rate of evaporation (liquid changing to vapor) equals the rate of condensation (vapor changing to liquid) on a molecular level such that there is no net inter-conversion. In simpler term, it means a condition where vapor (gas phase) and liquid are in equilibrium [1]. The formulation for vapor-liquid equilibrium for a multi-component system arises from the fact that the fugacity of species *i* in the vapor phase equal to the fugacity in the liquid phase.

$$f^v = f^l$$

$$y_i \phi_i P = \gamma_i x_i p_i' \quad (i=1, 2, \dots, N) \tag{1.1}$$

Where ϕ_i is the ratio of fugacity coefficients of component *i*, y_i and x_i are respectively vapor and liquid compositions, γ_i is the activity coefficient, p_i' is the vapor pressure and *P* is the total pressure.

The corresponding general vapor-liquid equilibrium equation for an ideal system reduces to

$$y_i p = x_i p_i' \quad (i=1, 2, \dots, N) \tag{1.2}$$

An important application of vapor-liquid equilibrium is the flash calculation. The name originates from the fact that a liquid at a pressure equal to or greater than its bubble point pressure “flashes” or partially evaporates when the pressure is reduced below the bubble point pressure, producing a two phase system of vapor and liquid in equilibrium [2, 3]. The appropriate laws for vapor-liquid equilibrium calculations include Raoult’s law, Dalton’s and Henry’s laws. Generally, flash calculations are calculations that are applied for processes where vapor and liquid are in equilibrium. A typical process that requires the application of flash calculation is when a feed stream (*F*) is separated into a vapor (*V*) and liquid (*L*) product as shown in Fig. 1.1. A very good example of this process is flash distillation which is partial vaporization without reflux. Possibility of vapor-liquid equilibrium data obtained at high pressure has been affirmed by [4].

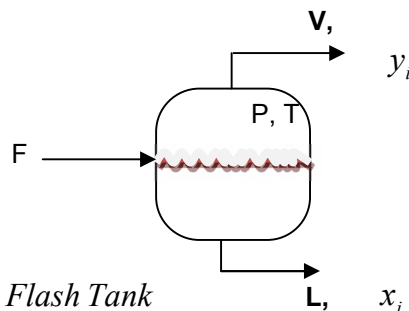


Fig. 1.1. Flash Tank

Since almost all the previous work on vapor-liquid equilibrium calculation are based on estimating only the vapor split and compositions, this new work has (in addition to these) unprecedentedly put forward a theory to obtain the pre-heat temperature with computer

implementation that can provide the results of vapor split, compositions, flow rates, enthalpy of vapor, average heat capacity of the feed and the pre-heat temperature for any two-phase vapor-liquid equilibrium flash process; thus the need for this model. It should be realized that an important aspect of vapor-liquid equilibrium flash calculation that has been previously neglected is the estimation of the pre-heat temperature. The pre-heat temperature is the temperature to which the feed must be subjected for a specific vapor split. The flash tank in Fig. 1.1 is just to show the material balance. In a typical flash distillation tank, the feed must be pre-heated in a heater before being led to a separator after the pressure might have been reduced via the throttling valve in order to maintain the equilibrium pressure and temperature. Previous authors have laid much emphasis on the equilibrium pressure and temperature which are the two important parameters to estimate the vapor split and compositions. In addition to this, this new model has made detail theory available to estimate this important parameter which is pre-heat temperature. This parameter is highly essential in plant design of flash tank.

This work is also targeted towards putting up a model on vapor-liquid equilibrium flash calculation that can give results essential in regulating the fabrication of vapor-liquid equilibrium flash distillation plant for a multi-component mixture. Furthermore, the theory puts forward here gives room for the estimation of the vapor pressures of the feed's components up to the critical points and this is another major advantage of these procedures. The significance and importance of considering feed's components critical points in vapor-liquid equilibrium flash calculation, which are previously lacking, have been provided in this work with detail explanation on how to regulate the final products. This model can therefore be said to give results essential in regulating the fabrication of a two-phase system flash distillation plant for multi-components feed. Other significances and importance of this work are explained in section (3) where the experimental and calculated results are presented and compared.

2. DESIGN METHODOLOGY FOR VAPOR-LIQUID EQUILIBRIUM (FLASH) CALCULATIONS

The theories put forward on process design for equilibrium flash calculation are discussed as follows:

2.1 Estimation of the Equilibrium Temperature Base on the Critical Temperature of Each Component of the Mixture

The critical temperature is the temperature where there is no change in the behavior of the gases no matter the alteration in the temperature [5]. The method employed entails the prediction of the flash point base on the lowest possible critical temperature of the components of the mixture (with respect to Wagner and extended Antoine equation) and therefore the calculation of the corresponding pressure requires to ensure vapor-liquid equilibrium at the predicted or estimated temperature. This is achievable since the time of ignition is dependent on the pressure [6]; and therefore the pressure requires for a specific flash point can be obtained.

It is important to note when this technique is employed that the flash temperature must not be higher than the lowest critical temperature of the feed's components. The critical temperatures of natural gas liquid components are presented in Table 2.1. Natural gas liquid can be stripped from natural gas by lean oil method described by Ridney and Parrish [7].

Table 2.1 Critical temperatures of natural gas liquid components

| Natural Gas Liquid Components | Critical Temperature (K) |
|-------------------------------|--------------------------|
| Ethane | 305.33 |
| Propane | 369.85 |
| N-Butane | 425.25 |
| I-Butane | 408.14 |
| N-Pentane | 469.80 |
| I-Pentane | 460.43 |
| Hexane | 507.90 |

Source: Polling et al (2001), the Properties of Liquid and Gases, 5th Edition, Appendix A, PP A.47-A.60

2.2 Estimation of the Flash Pressure

The major criterion that must be met in following the procedures entail in this work is that the flash pressure must lie between the bubble pressure and dew pressure. Thus, creates the need to calculate the vapor pressure of each component of the mixture, bubble point/pressure and dew point/pressure. The flash pressure is the pressure (total pressure) required to achieve equilibrium at a definite temperature (flash point). Various stages entails in estimating the flash pressure are discussed in the sub-sections that follow.

2.2.1 Calculation of the vapor pressure for each component using Wagner and extended Antoine equations

The major parameter needed in estimating the total pressure is the vapor pressure of each component. The other parameter is just the composition of each of the component in the feed. These are the two parameters needed to calculate bubble pressure and dew pressure (when Raoult's law holds) from which the flash pressure can be predicted.

Wagner equation represents the vapor pressure behavior of most substance over the entire liquid range and it is expressed as:

$$\ln p_{vp_r} = \frac{a\tau + b\tau^{1.5} + c\tau^{2.5} + d\tau^5}{T_r} \quad (2.1)$$

a, b, c and d are constants supplied by [8], T_r is the reduce temperature and τ is one minus reduce temperature. It is expedient to note that,

$$T_r = \frac{T_F}{T_C} \quad (2.2)$$

Where T_F and T_C are respectively flash temperature and critical temperature.

$$\tau = 1 - T_r \quad (2.3)$$

It is important to note that the exponential of Equation (2.1) gives the values of the reduce vapor pressure (p_{vp_r}). The value of the vapor pressure can be obtained by making use of the relation:

$$P'_i = P_{vp_i} \times P_{ci} \tag{2.4}$$

Where p'_i , p_{vp_i} and P_{ci} respectively denote vapor pressure, reduce vapor pressure and critical pressure of a particular component.

Extended Antoine equation covers enough temperature and pressure range even up to the critical points of some substances and it is expressed as;

$$\log_{10} p'_{vp_i} = A - \frac{B}{T + C - 273.15} + 0.43429x^n + Ex^8 + Fx^{12} \tag{2.5}$$

Where;

$$x = (T - t_o - 273.15) \tag{2.6}$$

Where A, B, C, E, F, n and t_o are constants which are readily available, T is the temperature in Kelvin. For the purpose of this work, Wagner and extended Antoine equations have been employed due to the fact that they are the two major equations that can be used to obtain the vapor pressure of most substances up to their critical points.

2.2.2 Bubble point/pressure calculation

This stage entails the calculation of the bubble pressure of the feed for the prediction of pressure corresponding to the predicted flash point. To determine the bubble pressure of the mixture, we make use of the general equation for vapor-liquid equilibrium expressed as;

$$y_i \phi_i P = \gamma_i x_i p'_i \quad (i = 1, 2, 3, \dots, N) \tag{2.7}$$

If the feed sample is of relatively low molecular force field, the condition could be subjected to ideal state with accurate results. Therefore, the ratio of fugacity coefficient Φ_i and activity coefficient γ_i are each equal to unity and Equation (2.7) becomes;

$$y_i P = x_i p'_i \tag{2.8}$$

Recall that $y_i P = p_i$ (2.9)

Equation (2.8) therefore becomes,

$$P_i = x_i p'_i \tag{2.10}$$

Where P_i , P, and P_i are respectively vapor pressure, total pressure and partial pressure. It should be recalled that the summation of partial pressure of all components in a mixture equals the total pressure that is;

$$\sum P_i = P \tag{2.11}$$

So that; $\sum x_i P'_i = P_{bubble}$ (2.12)

Thus, the value obtained from Equation (2.12) gives the bubble pressure of the mixture. It is expedient to take note that the value of x_i in Equation (2.12) is taken equivalent to be molar composition (z_i) of each component in the feed for bubble pressure calculation. That is, Equation (2.12) could be written as;

$$\sum z_i P_i' \quad (2.13)$$

2.2.3 Dew point/pressure calculation

To calculate the dew point of the mixture, a suitable equation has to be derived from Equation (2.7). Equation (2.7) can be rewritten as;

$$x_i = \frac{y_i \phi_i P}{\gamma_i P_i'} \quad (2.14)$$

Since in flash calculation $\sum_i x_i = 1$ for liquid phase, we have;

$$1 = \sum_i \left(\frac{y_i \phi_i P}{\gamma_i P_i'} \right) \quad (2.15)$$

From Equation (2.15), the expression for dew pressure is given as,

$$p = \frac{1}{\sum_i (y_i \phi_i / \gamma_i P_i')} \quad (2.16)$$

For an ideal condition, Equation (2.16) becomes,

$$p = \frac{1}{\sum_i \left(\frac{y_i}{P_i'} \right)} \quad (2.17)$$

Also, as it was done in the case of bubble pressure calculation, the value of y_i in Equation (2.17) is equivalent to that of z_i , so that Equation (2.17) can be written as;

$$P_{dew} = \frac{1}{\sum_i \left(\frac{z_i}{P_i'} \right)} \quad (2.18)$$

2.2.4 Prediction of the flash pressure from the result of the bubble pressure and dew pressure

The major criteria for the validity of this vapor-liquid equilibrium (flash) calculation as stated earlier is that the flash pressure must lie between the bubble pressure and dew pressure. Hence, the need to carry out bubble pressure and dew pressure calculations. These steps help to predict a suitable pressure for the flash calculation at a specific flash point.

The predicted flash temperature will correspondingly be an equilibrium temperature once the pressure estimated (by bubble pressure and dew pressure calculations) via this temperature lies between the bubble pressure and dew pressure; and vice versa.

2.3 Calculation of the Phase Equilibrium Constant for Each Component of the Mixture

With reference to general equation for vapor-liquid equilibrium which is expressed as,

$$y_i \phi_i P = \gamma_i x_i P_i'$$

We can write,

$$\frac{y_i}{x_i} = \frac{\gamma_i P'_i}{\phi_i P} = k_i \quad (2.19)$$

Where k_i denotes phase equilibrium constant of a component i . Base on Raoult's law, Equation (2.19) becomes,

$$K_i = \frac{P'_i}{P} \quad (2.20)$$

Where p is the predicted flash pressure (total pressure) and p'_i is the obtained vapor pressure of component i via Wagner equation or extended Antoine equation.

2.4 Calculation of the Vapor Split (Percentage Vaporized) on Flashing by Solving Iterative Rachord-Rice Equation, Liquid Composition (x_i) and Vapor Composition (y_i)

One of the major objectives of the flash calculation is towards the optimum vapor split. One of the major factors that determine the percentage vaporized is actually the flash pressure which varies inversely with the percentage vaporized. Obtaining an expression for relating vapor split with composition and phase equilibrium constant entails taking a material balance around an exemplified flash distillation process comprising a two phase equilibrium process as depicted in Fig. 1.1. For each of the N_C components, the material balance is;

$$F z_i = L x_i + V y_i \quad (2.21)$$

Since vapor and liquid are in equilibrium, Equation (2.19) can be written as,

$$y_i = k_i x_i$$

By substituting $y_i = k_i x_i$ in Equation (2.21),

$$F z_i = L x_i + V k_i x_i \quad (2.22)$$

Making x_i the subject of formula in Equation (2.22) gives;

$$x_i = \frac{FZ_i}{L + V k_i} \quad (2.23)$$

Since $L=F-V$, substituting for L in Equation (2.23) gives;

$$x_i = \frac{FZ_i}{F - V + V K_i} \quad (2.24)$$

so that;

$$x_i = \frac{Z_i}{1 + \frac{v}{F}[k_i - 1]} \quad (2.25)$$

Also, by substituting $x_i = \frac{y_i}{k_i}$ in Equation (2.21) and making y_i the subject of formula for further simplification as used in deriving equation (2.23) gives,

$$y_i = \frac{Z_i k_i}{1 + \frac{v}{F}[k_i - 1]} \quad (2.26)$$

Where V/F denotes vapor split (percentage of the feed vaporized). It is a criteria for a valid vapor-liquid equilibrium calculation that $\sum_i y_i = \sum_i x_i = 1$. So that equation (2.23) can be written as;

$$\sum_{i=1}^{Nc} x_i = \sum_{i=1}^{Nc} \frac{Z_i}{1 + \frac{v}{F}(k_i - 1)} \quad (2.27)$$

To obtain a monotonic function equation in V/F , we write,

$$\sum_i (y_i - x_i) = 0 \quad (2.28)$$

So that by substituting Equations (2.24) and (2.26) into Equation (2.28), we have,

$$\sum_i \frac{z_i (k_i - 1)}{1 + \frac{v}{F}[k_i - 1]} = 0 \quad (2.29)$$

Equation (2.29) is the so called Rachord-Rice equation and can be solved to obtain vapor split by either trial and error method or Newton- Raphson method. A physical solution must satisfy $0 \leq V/F \leq 1$.

2.6 Estimation of the Pre-Heat Temperature for Specific Vapor Split

In almost all the previous work on vapor-liquid equilibrium calculations, especially flash calculations, the major aims are to calculate the vapor split and compositions. These aims have been extended in this work to involve the prediction or estimation of the pre-heat temperature by modification of the procedure given by McCabe et al. [1].

Pre-heat temperature is the temperature to which the feed would be subjected for a specific vapor split. Most of the previous work emphasis has been on using flash temperature to estimate only the compositions and vapor split without predicting the pre-heat temperature. In practice, the feed has to be pre-heated to a specific temperature before being regulated to an equilibrium temperature. Thus, creates the need to estimate the pre-heat temperature which is an important parameter in plant design. An enthalpy balance is made using flash temperature in order to determine the pre-heat temperature. This entails calculations of the heats of vaporization at the flash temperature and the average heat capacities of the liquid from the flash point to a predicted temperature range. The unprecedented theories and explanations are given in the following sub-sections on different stages involve in the estimation of the pre-heat temperature for a specific vapor-split.

2.6.1 Calculation of the heat of vaporization at the flash point

The expression for estimating the heat of vaporization of a fluid at a specific temperature as suitable for this theory is;

$$\frac{\Delta H_V}{RT_C} = 7.08[1 - T_r]^{0.354} + 10.95w(1 - T_r)^{0.456} \quad (2.30)$$

Where ΔH_V the needed heat of vaporization, w is the acentric factor (constant for all compounds) and R is the gas constant. The unit of measurement of heat of vaporization in equation (2.30) is determined by the unit of temperature and gas constant used. It is important to take note that the criteria for the appropriation of Equation (2.31) is that the range of the reduce temperature of the substance should be between 0.6 and 0.99, that is, $0.6 < T_r < 1.0$.

2.6.2 Calculation of the heat capacities for each component over a predicted temperature range from the flash point

The pre-heat temperature is primarily expected to be above the flash point for most flash distillation plant design. The molar heat capacities for each component in the mixture are therefore calculated from the flash point to a predicted temperature of about 100°C or less above the flash point. The expression for calculating the molar heat capacities of liquid and gases; the heat capacity at a specific temperature is expressed as:

$$\frac{C_p^o}{R} = a_o + a_1T + a_2T^2 + a_3T^3 + a_4T^4 \quad (2.31)$$

Where a_o , a_1 , a_2 , a_3 , and a_4 are constants, provided by (5).

2.6.3 Calculation of the average heat capacity for each of the feed's components

The average heat capacity is needed to be calculated for each of the components of the mixture. This is easily obtained from the average value of the heat capacities over the entire temperature range from the flash point.

$$\overline{C_{Pi}} = \frac{\sum_i C_{Pi}^o}{N_{C_{Pi}}} \quad (2.32)$$

$N_{C_{Pi}}$ is the total number of heat capacities for each component over the entire temperatures' range. The components average molar heat capacities are used to predict expression for the average molar heat capacity of feed as given in the next section.

2.6.4 Calculation of the Average Molar Heat Capacity of the Feed ($\overline{C_{pf}}$)

The average molar heat capacity of the feed is obtained from the feed's composition and average heat capacities of the feed's component. This relation is expressed as:

$$\overline{C_{pf}} = \sum_{i=1}^{N_c} \overline{C_{pi}} Z_i \quad (2.33)$$

$\overline{C_{pi}}$ is the average molar heat capacity of each of the feed's components.

2.6.5 Calculation of the enthalpies of the liquid and vapor phases

The enthalpy of the vapor phase can be predicted from the estimated heat of vaporization and composition of each component in the vapor phase. This relation is given by,

$$H_v = f \left[\sum_{i=1}^{N_c} [y_i \times \Delta H_{v_i}] \right] \quad (2.34)$$

f is the obtained vapor split and H_{v_i} is the heat of vaporization of each component at the flash point.

It is expected that the enthalpy of the liquid phase should be zero since the conversion is from the liquid phase to the vapor phase.

2.6.6 Obtaining the preheat temperature

The pre-heat temperature, depicting the final temperature to which the feed must be heated for a definite vapor split can be estimated in terms of the average molar heat capacity of the feed and the enthalpy of the vapor phase. This relation is given by,

$$H_v = \bar{C}_p [T_o - F_T] \quad (2.35)$$

Equation (2.35) can be expressed in term of pre heat temperature as;

$$T_o = \frac{H_v}{\bar{C}_p} + F_T \quad (2.36)$$

F_T denotes flash temperature.

2.7 Calculation of the Vapor and Liquid Flow Rates (v_i and l_i)

For complete design methodology for vapor-liquid equilibrium calculations, it is essential to estimate each component flow rates in liquid and vapor phases. These can be obtained by dividing Equation (2.21) by F so that;

$$z_i - \frac{L}{F} x_i = \frac{V}{F} y_i$$

Therefore,

$$v_i = y_i \times \frac{V}{F} \quad (2.37)$$

$$l_i = x_i \times \left(1 - \frac{V}{F} \right) \quad (2.38)$$

3. RESULTS AND DISCUSSION

The results of these theories applied for natural gas liquid (a mixture of hydrocarbon compounds) shows that a natural gas liquid subjected to a temperature of 411.07 k forms a two phase vapor-liquid equilibrium system at a temperature of 304k and pressure of 3.8bar to give 72.8% of the feed in the vapor phase with average feed molar heat capacity of 103.56 j/mol k and corresponding 11089.09J as the enthalpy of vapor. It should be noted that the theory put forward here is appropriate for any mixture of hydrocarbon compounds

and other molecules of relatively uncomplicated molecular force field. We have made use of natural gas liquid as the feed because it is a multi-components mixture of light hydrocarbon compounds. Any other multi-components mixture of hydrocarbon compounds or other molecules of relatively uncomplicated molecular force fields could as well be considered as the feed in this model.

The interface (form) for the computer implementation of the calculations involved is:

It has been found that equilibrium pressure is inversely proportional to the vapor split (as depicted in Fig. 3.3).

The interpretation of Figs. 3.1 and 3.2 is that high separation can be obtained at a low equilibrium pressure but high flash temperature and vice versa (vapor split depicts the percentage of the feed in the vapor phase). These two conditions can be varied especially flash pressure to regulate the quantities and qualities of the final products.

The results of the vapor and liquid compositions and their respective molar flow rates are presented in Table 3.1.

For the estimation of the preheat temperature, the results of reduced temperature (T_r), heat of vaporization (H_v) and average heat capacity (\bar{C}_{pi}) for each component of the feed with the values of the acentric factors (w) are shown in Table 3.2. All these results are obtained from appropriate equations put forward in the methodology.

Application of Equation (2.36) gives the value of pre-heat temperature to be 411.07k from the values of average heat capacity of feed which is 103.56J/mol k and 11089.09J as the enthalpy of vapor.

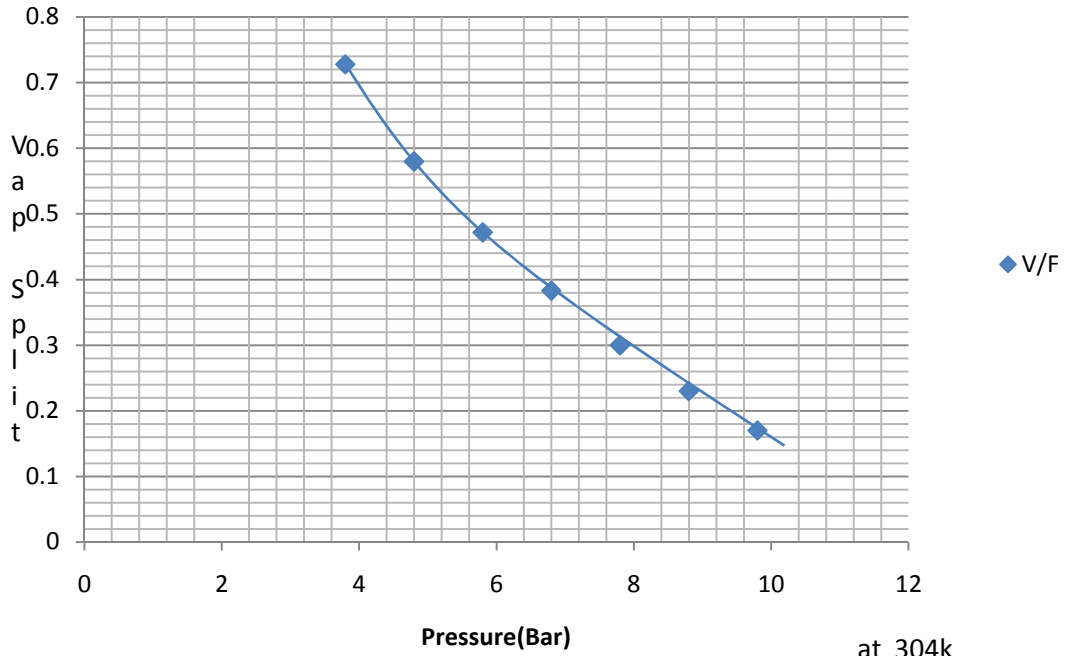


Fig. 3.1 Variation of vapor splits with pressures at constant temperature

Vapor splits at different equilibrium temperatures are shown in Fig. 3.4 below:

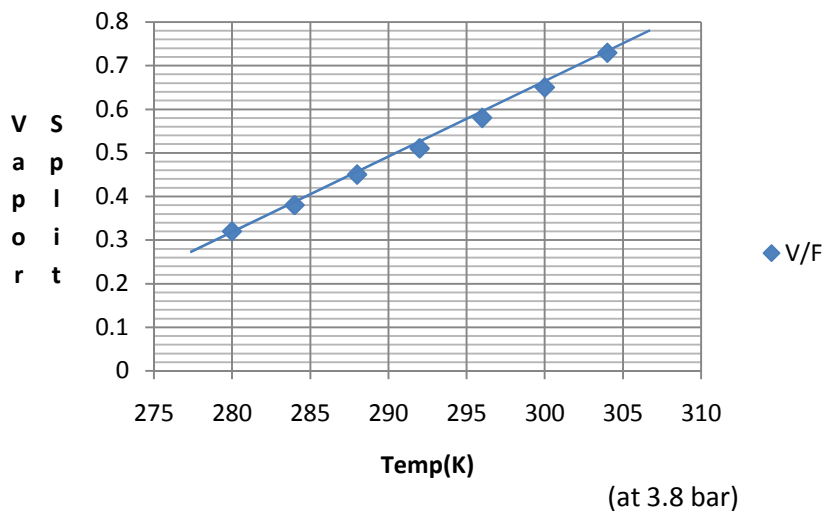


Fig. 3.2 Variation of vapor split with temperature at constant pressure

Table 3.1 Results of the liquid phase compositions (x_i), vapor phase compositions (y_i), vapor molar flow rates (v_i) and liquid molar flow rates (l_i)

| Feed's components | Z_i | K_i | x_i | y_i | v_i | l_i |
|-------------------|-------|-------|--------------|--------------|--------|---------|
| Ethane | 0.14 | 12.47 | 0.015 | 0.1867 | 0.1359 | 0.00408 |
| Propane | 0.25 | 4.77 | 0.0668 | 0.3185 | 0.2317 | 0.0182 |
| N-Butane | 0.05 | 0.77 | 0.0601 | 0.0462 | 0.0336 | 0.0163 |
| I-Butane | 0.30 | 1.09 | 0.2816 | 0.3069 | 0.2234 | 0.0766 |
| N-Pentane | 0.13 | 0.22 | 0.3008 | 0.0662 | 0.0482 | 0.0818 |
| I-Pentane | 0.12 | 0.30 | 0.2447 | 0.0734 | 0.0534 | 0.0666 |
| Hexane | 0.01 | 0.07 | 0.031 | 0.0022 | 0.0016 | 0.0084 |
| | | | $\sum x_i=1$ | $\sum y_i=1$ | | |

Table 3.2 The results of the reduced temperature (T_r), heat of vaporization (H_{vi}) and average heat capacity (\bar{C}_{pi}) for each component of the Feed with the values of the acentric factors(w)

| Feed's components | Acentric factor(w) | T_r | $H_{vi}(J)$ | \bar{C}_{pi} (J/kmol) |
|-------------------|--------------------|--------|-------------|-------------------------|
| Ethane | 0.099 | 0.9956 | 2854.19 | 58.81 |
| Propane | 0.152 | 0.8220 | 14149.08 | 83.65 |
| N-butane | 0.200 | 0.7149 | 20423.89 | 111.52 |
| I-butane | 0.186 | 0.7448 | 18522.02 | 110.25 |
| N-pentane | 0.252 | 0.6471 | 25831.00 | 136.03 |
| I-pentane | 0.229 | 0.6603 | 24362.89 | 137.04 |
| Hexane | 0.300 | 0.5985 | 30793.66 | 163.86 |

This work is primarily meant to provide means of estimating pre-heat temperature in vapor-liquid equilibrium flash calculation which is an aspect that has been neglected by most of the previous authors on vapor-liquid equilibrium flash calculation. For example, [9,10,11,12,13, 14,15,16], among others, based their vapor-liquid equilibrium flash calculations on estimating only the vapor split and compositions. McCabe et al. [1] unprecedentedly put forward a model for predicting pre-heat temperature but failed to provide means to obtain heat capacities and heat of vaporizations of the feed's components which are respectively required to estimate average heat capacity of the feed and enthalpy of vapor. In other words, they only gave experimental results for these parameters. This work has successfully put forward the model for estimating these important parameters which are essential for estimating the pre-heat temperature and also for every other result obtainable in vapor-liquid equilibrium flash calculation. Thus, this work provides a complete model for vapor-liquid equilibrium flash calculation.

Since Smith et al. [11] have affirmed the validity of vapor- liquid equilibrium flash calculation of mixture with relatively uncomplicated molecular force fields based on ideal state to give almost the same results as for non-ideal state, the model predicted here is meant for mixture with relatively low molecular force fields which provides approximate results with respect to non-ideal state . All light hydrocarbon compounds fall in this category. Thus, this theory is appropriate for any multi-components hydrocarbon mixture and other molecules of relatively uncomplicated molecular force fields (which can be explained in term of relative molecular masses). This model is therefore highly appropriate for industrials' multi-components separations and the computer implementation put forward will be of great use to industries

and also for academics' purpose. This computer implementation has been tested and found to give accurate results with respect to all the calculated results on vapor-liquid equilibrium flash calculation.

To validate this model, we applied the theory put forward here to carry out vapor-liquid equilibrium flash calculation carried out by McCabe et al. [1] for a mixture of light hydrocarbon compounds containing hexane, heptane and octane. The experimental results obtained are presented below:

| Feed | z_i | k_i | x_i | y_i | H_{vi} (cal/mol) | $\overline{C_{pi}}$ (cal/mol $^{\circ}c$) |
|---------|-------|-------|------------------|--------------|--------------------|--|
| Hexane | 0.33 | 2.23 | 0.190 | 0.424 | 6370 | 62 |
| Heptane | 0.37 | 1.01 | 0.368 | 0.372 | 7510 | 70 |
| Octane | 0.30 | 0.462 | 0.443 | 0.204 | 8560 | 78 |
| | | | $\sum x_i=1.001$ | $\sum y_i=1$ | | |

The vapor split here is 0.6. The enthalpy of vapor and average heat capacity of the feed are respectively 4345 cal and 69.8 cal/mol $^{\circ}C$. The pre-heat temperature is 167 $^{\circ}C$.

The calculated results obtained via this model are presented below:

| Feed | z_i | k_i | x_i | y_i | l_i | v_i |
|---------|-------|-------|--------------|--------------|--------|--------|
| Hexane | 0.33 | 2.379 | 0.181 | 0.430 | 0.0724 | 0.258 |
| Heptane | 0.37 | 1.004 | 0.369 | 0.370 | 0.1476 | 0.222 |
| Octane | 0.30 | 0.447 | 0.450 | 0.199 | 0.1800 | 0.1194 |
| | | | $\sum x_i=1$ | $\sum y_i=1$ | | |

Other results via this model fall in the range provided below:

| Feed | Omega (w) | T_r | H_{vi} (cal/mol) | $\overline{C_{pi}}$ (cal/mol $^{\circ}c$) |
|---------|-----------|-------|--------------------|--|
| Hexane | 0.30 | 0.74 | 6300 | 61.8 |
| Heptane | 0.35 | 0.70 | 7400 | 69.5 |
| Octane | 0.399 | 0.66 | 8500 | 77.0 |

The vapor split here is also 0.6. The enthalpy of vapor and average specific heat capacity of the feed are respectively 4283.1cal and 69.21cal/mol $^{\circ}C$. The pre-heat temperature via this model is therefore 166.89 $^{\circ}C$.

There are quite glaring similarities in the two results presented above. The calculated values of the heat of vaporizations can be made closer by using critical temperatures in whole numbers. The new model gives in addition the values of the liquid and vapor flow rates which are important parameters for flash distillation plant design. This new model also avoids the use of charts to estimate vapor pressure but provide equation that can give vapor pressure up to the critical points of the feed's components. This also enables the values of the equilibrium constants to be obtained up to three or more decimal places unlike chart like De-priester chart that gives the value of vapor pressure in whole number. This also helps to increase the accuracy of the results. The computer implementation unprecedentedly put forward can provide the results of phases' compositions and flow rates, vapor split, enthalpy of vapor, average heat capacity of the feed and pre-heat temperature. It is therefore termed

flash calculator. It has been made to be software that can be installed. It has been applied and found accurate for the results presented in this paper including for experimental results using experimental parameters. This model can therefore be referenced as complete model that unprecedentedly put forward a theory that can supply all the results obtainable in vapor-liquid equilibrium calculation since some theories are lacking in previous models. This model can therefore be said to give results essential in regulating the fabrication of a two-phase system flash distillation plant for multi-component feed.

4. CONCLUSION

The procedures put forward in this work are appropriate for any mixture of hydrocarbon compounds (with their isomers) and other molecules of relatively uncomplicated molecular force field. The condition of low pressure will favor more components in the vapor phase. Thus, this condition is most suitable when each component of the mixture is needed to be treated or separated; although, as already explained, the conditions of the process (both temperature and pressure), for example equilibrium pressure at a specific equilibrium temperature or equilibrium temperature at a specific equilibrium pressure, can be varied to regulate or determine the quantity of the resulted vapor split. Also, since most of the extraction processes designed for separating natural gas liquid are targeted towards obtaining certain component of the mixture, the method put forward here will be highly essential for processing all of the components of the natural gas liquid, even as the demand for them increases. This work can be applied to aid plant's fabrication of any two-phase vapor-liquid equilibrium process.

In estimating the pre-heat temperature as put forward in this work, the range of temperature predicted for estimating the heat capacity of the feed's components can be reduced in order to save time and especially for texts use. This can only increase the accuracy of the result.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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