RESEARCH ARTICLE OPEN ACCESS

Shortcut Design Method for Multistage Binary Distillation via MS-Excel

Mr. S. B. Dongare[a], Mr. A.C.Shende[a], Dr.V.N.Ganvir[a], Dr. G.M.Deshmukh[a]
[a]*Laxminarayan Institute of Technology, Rashtrasant Tukadoji Maharaj Nagpur University,*
Nagpur-440033, India.

ABSTRACT

Multistage distillation is most widely used industrial method for separating chemical mixtures with high energy consumptions especially when relative volatility of key components is lower than 1.5. The McCabe Thiele is considered to be the simplest and perhaps most instructive method for the conceptual design of binary distillation column which is still widely used, mainly for quick preliminary calculations.

In this present work, we provide a numerical solution to a McCabe-Thiele method to find out theoretical number of stages for ideal and non-ideal binary system, reflux ratio, condenser duty, reboiler duty, each plate composition inside the column.

Each and every point related to McCabe-Thiele in MS-Excel to give quick column dimensions are discussed in details.

Keywords: Multistage distillation; McCabe-Thiele Method; Non-ideal System; Relative volatility

I. INTRODUCTION

More than 90 years ago, McCabe-Thiele developed a creative graphical solution technique based on Lewis assumptions of constant molar overflow for the rational design of distillation column.[1]

There are two ways to do distillation calculations by McCabe-Thiele method. One is graphical method (by hand and time consuming), and other way is by using any other commercial simulation software. It is costly and require license. A third alternative is presented here: Merging the graphical and manual computational methods so that the inaccuracies of the former are compensated for by the speed of the computations. The calculations can be run by any spreadsheet program, such as Microsoft Excel, eliminating the need for employing expensive simulation software and for laboring over hand calculations. Further, the time involved from a programmer's point of view is no more (or considerably less) than that required to learn how to use a commercial simulation package.

The method presented here is easy to learn, and offers a quick way to make preliminary estimates of the tower diameter and height, number of stages, energy consumption, and reflux ratio. Although the calculation procedure is intended for binary systems, ternary systems can also be modeled if the third component is less than 10% by volume and its volatility is not drastically different from the those of the remaining two components.

II. SPREADSHEET CALCULATION PROCEDURE

While performing the distillation design calculation, it is necessary to do mass balance around the distillation column (i.e. by knowing feed, distillate and residue conditions), is determining the vapor/liquid equilibrium (VLE) data. Raoult's law is used to calculate the saturation pressure for the pure components [2]. Since most systems are non-ideal, the Wilson equation is then applied to determine the liquid and vapor compositions [3]. This equation includes the activity coefficients for a mixture, making it suitable for non-ideal systems. A water/Acetic Acid system is used to illustrate the overall method.

III. APPLY RAOULT'S LAW AND THE WILSON EQUATION

Use Raoult's law to find the saturated vapor pressure for each component. Published data are available for various compounds. The saturated vapor pressure of each component is expressed as:

$$\ln P_i^s = A_i - \frac{B_i}{C_i + T} \qquad (1)$$

where, P_{1sat} is the saturated vapor pressure of component 1 (Pa), T is the temperature (K), and A, B, and C are the Raoult's law constants for each compound[4]. The corresponding parameter values for Acetic Acid and water are given in Table 1. To calculate the saturation pressure of a

component, simply substitute the value of the temperature. In these calculations,
1 refers to Water and 2 is for Acetic Acid.

Table 1- Raoults Law constants for Water & Acetic Acid

Compound	A	B	C
Water	18.5882	3984.52	233.43
Acetic Acid	18.47233	4457.83	258.46

The liquid and vapor mole fractions of Water (x_1 and y_1, respectively) are found using the total system pressure, P_{total}:

$$x_1 = P_{1sat}/(P_{1sat} + P_{2sat}) \quad (2)$$

$$y_1 = (x_1 P_{1sat})/P_{total} \quad (3)$$

For an ideal system, these equations will determine the VLE data needed to estimate the column dimensions.

When a liquid contains dissimilar polar species, particularly those that can form or break hydrogen bonds, the ideal liquid solution assumption is almost always invalid and the regular solution theory is not applicable. Non ideal solution effects can be incorporated into K-value formulations, therefore VLE calculations are carried out by using the activity coefficients for the liquid which are calculated to correct the equilibrium constant. At present there are at least four different types of correlation for the predication of activity coefficients in chemical systems that are normally used: Wilson, NRTL, UNIQUAC and UNIFAC.[3]

For non-ideal mixture or azeotropic mixture additional variable γi (activity coefficient) appears in vapor-liquid equilibrium equation.

$$y_i = \gamma i * \frac{\text{Pi sat}}{\text{Ptotal}} * \text{Xi} \quad (4)$$

Where represents degree of deviation from reality. When $\boldsymbol{\gamma i}$ =1, the mixture is said to be ideal which simplifies the equation to Raoult's law. For non-ideal mixture $\boldsymbol{\gamma i} \neq 1$, exhibits either positive deviation from Raoult's law ($\boldsymbol{\gamma i} > 1$), or negative deviation from Raoult's law ($\boldsymbol{\gamma i} < 1$).

The prediction of liquid phase activity coefficient is most important for design calculation of non-ideal distillation. Before calculating vapor-liquid equilibrium of non-ideal mixture, the activity coefficient of each component must be calculated. There is several excess energy models to calculate the activity coefficient for multicomponent systems, the most important models are of (Wilson, NRTL, UNIFAC, and UNIQUAC). In all these models, the model parameters are determined by fitting the experimental data of binary mixtures. Each one of these models has advantages and disadvantages. There is no general model which has a good representation of all azeotropic mixtures. The selection of appropriate model for a given mixture is based on three characteristics, which are temperature, pressure and composition. If inappropriate model is selected, the design and simulation of the process will not work well.

Based on molecular considerations, Wilson (1964) presented the following expression for the excess Gibbs energy of a binary solution:

$$\frac{g^E}{RT} = -x_1 \ln(x_1 + A_{12}x_2) - (x_2 + A_{12}x_1) \quad \text{…………………..(10)}$$

The Activity coefficients derived from this equations are

$$\ln \gamma_1 = -\ln\left(x_1 + A_{12}x_2\right) + x_2\left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{x_2 + A_{21}x_1}\right) \quad \text{…………….(11)}$$

$$\ln \gamma_1 = -\ln\left(x_2 + A_{21}x_1\right) - x_1\left(\frac{A_{12}}{x_1 + A_{12}x_2} - \frac{A_{21}}{x_2 + A_{21}x_1}\right) \quad \text{……………(12)}$$

In Eq. (10) the excess Gibbs energy is defined with reference to an ideal solution in the sense of Raoults Law; Eq(10) obeys the boundary conditions that g^E vanishes as either x_1 or x_2 becomes zero. [2]

Wilson's equation has two adjustable parameters. A12 and A21. in Wilson's derivation, these are related to the pure-component molar volumes and to characteristics energy differences by

$$A_{12} = \frac{v_2^L}{v_1^L}\exp\left(-\frac{\lambda_{21} - \lambda_{11}}{RT}\right) \quad \text{…………….(13)}$$

$$A_{21} = \frac{v_1^L}{v_2^L} \exp\left(- \frac{\lambda_{21} - \lambda_{22}}{RT} \right)$$

………………(14)

Where v_i is the molar liquid volume of pure component i and λ_{ij} are energies of interaction between the molecules designated in the subscripts. To a fair approximation, the differences in the characteristic energies are independent of temperature, at least over modest temperature intervals. Therefore, Wilson's equation gives not only an expression for the activity coefficients with temperature. This may provide a practical advantage in isobaric calculations where the temperature varies as the composition changes. For accurate work, $(\lambda_{12} - \lambda_{11})$ and $\ln P^s = A - \frac{B}{T + C}$ should be considered temperature-dependent but in many cases this dependence can be neglected without serious error. Wilson's equation appears to provide a good representation of excess Gibbs energies for a variety of miscible mixtures.

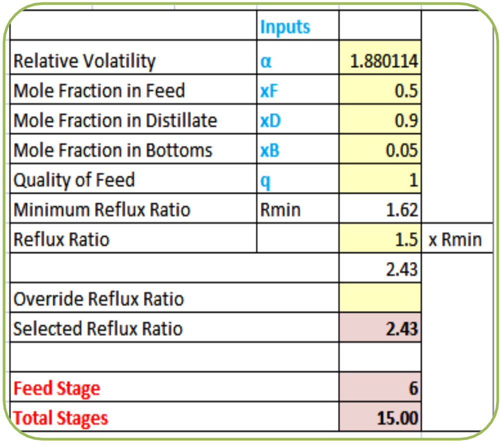
Table 3-Spreadsheet for the tabulation of VLE data

Temp (^{0}C)	Vapor Pressure (mm Hg)		Partial Pressure Pressures (mm Hg)		Sum Pp/Ptotal	Water Mole Fractions		Acetic Acid Mole Fractions	
	Water	Acetic Acid	Water	Acetic Acid		x1	y1	x2	y2
99.866	760	416.3959	760	0	1	1	1	0	0
100.77	785.161451	429.7352	734.1277	25.8723	1	0.935002	0.965958	0.064998	0.034042
101.68	811.012368	443.4313	711.7857	48.21433	1	0.877651	0.93656	0.122349	0.06344
102.59	837.567355	457.4914	689.0826	70.9174	1	0.822719	0.906688	0.177281	0.093312
103.50	864.841221	471.9232	664.4168	95.58319	1	0.768253	0.874233	0.231747	0.125767
105.32	921.60585	501.9327	607.2258	152.7742	1	0.658878	0.798981	0.341122	0.201019
106.24	951.127259	517.5262	574.6344	185.3656	1	0.604161	0.756098	0.395839	0.243902
109.88	1077.17407	584.0134	421.9733	338.0267	1	0.391741	0.555228	0.608259	0.444772
112.61	1180.52371	638.4317	290.1247	469.8753	1	0.245759	0.381743	0.754241	0.618257
114.43	1253.87266	677.0083	196.5885	563.4115	1	0.156785	0.258669	0.843215	0.741331
117.16	1370.91837	738.4991	50.14049	709.8595	1	0.036574	0.065974	0.963426	0.934026
118.07	1411.87783	760	-1.8E-12	760	1	-1.3E-15	-2.4E-15	1	1

IV. CALCULATE VLE DATA

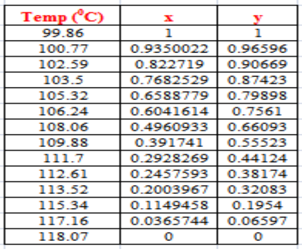
Table 3 presents the spreadsheet for the water/Acetic Acid binary system (only the beginning, middle and ending sections are shown). The program also includes cells for the Wilson coefficients and those for Raoult's law, which are not shown in Table 3. The temperature values between boiling ranges of components are chosen by the programmer. The number of these values chosen determines, of course, the number of data points. All other entries in the table are either constants, or functions of constants and the inputted temperature. To find the partial pressures of both components (Columns 4 and 5), the saturated vapor pressures are needed at a given temperature (Columns 2 and 3). The saturated vapor pressures are calculated using Raoult's law and the partial pressures by applying the Wilson equations. Since the total pressure is predetermined, a test column is set up in which the total pressure (the sum of the partial pressures) is divided by the actual total pressure at that stage (Column 6). When this value in Column 6 approaches unity (within a given tolerance) the correct temperature has been found. Thus, once values of x1 are chosen, the only variable is the temperature (Column 1).

Table 4- Spreadsheet of Input details



	Inputs		
Relative Volatility	α	1.880114	
Mole Fraction in Feed	xF	0.5	
Mole Fraction in Distillate	xD	0.9	
Mole Fraction in Bottoms	xB	0.05	
Quality of Feed	q	1	
Minimum Reflux Ratio	Rmin	1.62	
Reflux Ratio		1.5	x Rmin
		2.43	
Override Reflux Ratio			
Selected Reflux Ratio		**2.43**	
Feed Stage		**6**	
Total Stages		**15.00**	

Table 5 – Calculated Vapor-Liquid VLE data



Temp (^{0}C)	x	y
99.86	1	1
100.77	0.9350022	0.96596
102.59	0.822719	0.90669
103.5	0.7682529	0.87423
105.32	0.6588779	0.79898
106.24	0.6041614	0.7561
108.06	0.4960933	0.66093
109.88	0.391741	0.55523
111.7	0.2928269	0.44124
112.61	0.2457593	0.38174
113.52	0.2003967	0.32083
115.34	0.1149458	0.1954
117.16	0.0365744	0.06597
118.07	0	0

V. FLOW DIAGRAM OF MS-EXCEL SPREADSHEET-

Fig. 1 shows the stepwise calculation procedure for this spreadsheet. Spreadsheet snapshot of input values such as Relative Volatility, Mole fraction of feed, Distillate & Residue and calculates VLE data is shown in Table 4 & 5 reply.

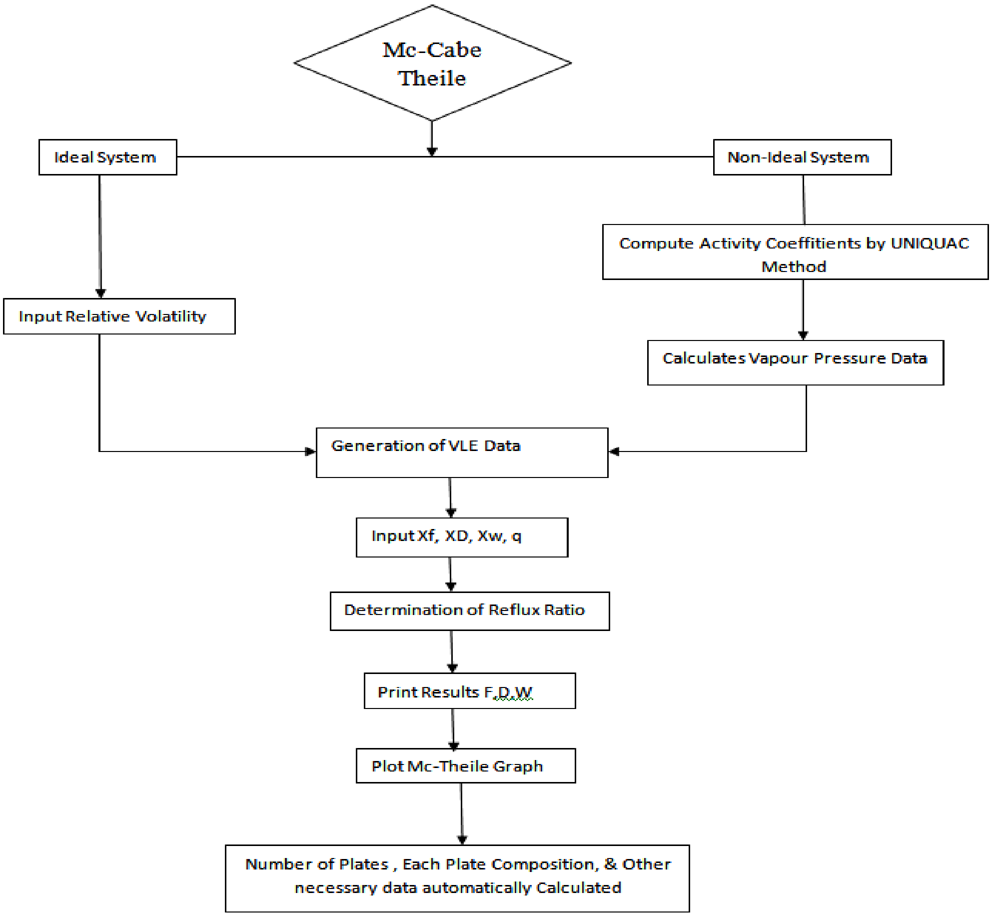


Fig. 1- Flow diagram of Excel Spreadsheet

VI. DETERMINE THE THEORETICAL NUMBER OF STAGES -

The theoretical number of stages is calculated using the McCabe- Thiele method (Fig. 2). The following algorithm is used to generate the appropriate data points and “construct” the diagram (xD is the distillate composition):

1. Start at the y = x line for the distillate conditions (x, y) = (x_D, x_D).
2. Follow the constant y line to the VLE line point (x, y) = (x_{VLE}, x_D).
3. There are two options. For total reflux, follow the constant x $_{VLE}$ line to the y = x line for total reflux to the point (x, y) = (x_{VLE}, x_{VLE}). Alternatively, follow the x_{VLE} line to the minimum or optimum reflux line: y = mx + b to the point (x, y) = (x_{VLE}, m x_{VLE} + b).
4. Repeat the algorithm for the new data point set defined in Step 3.

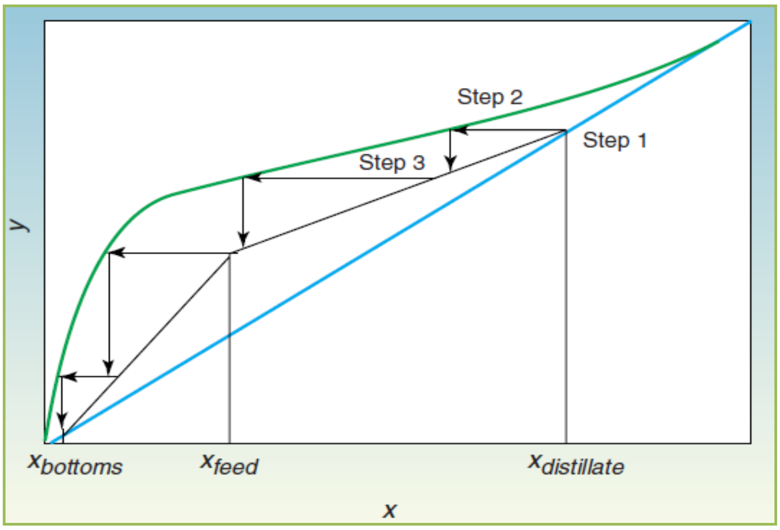


Fig 2-McCabe-Thiele diagram for determining the number of stages in the rectifying and stripping sections of a distillation column

VII. COLUMN SPECIFICATIONS

Table 4 presents the feed, distillate and bottom specifications for the column, as well as other operating parameters. A reflux ratio of 1.5 times the minimum reflux ration was chosen arbitrarily. Table 4 calculates the flow conditions, based on the mass balance of the system. Water is referred to as the "graphed" component to differentiate it from the other component (Acetic Acid) used in the calculations. These three tables (Tables 4, and 5) contain all the data needed to define the system, now that the VLE data are determined. Next, calculations are performed to find the minimum number of stages.

Minimum number of stages

The minimum number of ideal stages, which occurs at total reflux, is calculated using the algorithm presented before. Table presents the results for the water/Acetic Acid system. The values for the first row (x, y) are (x_D, y_D), and for all subsequent rows are (x_{VLE}, y_{VLE}), based on the previous x and y values, which are calculated using the equations.. This spreadsheet was set up to calculate compositions for 15 stages. This number is usually more than sufficient to accommodate most distillation columns. The calculations generated a value of x = 0.90 for Stage 1, which is a bottoms of essentially equal to zero as shown in fig.3.

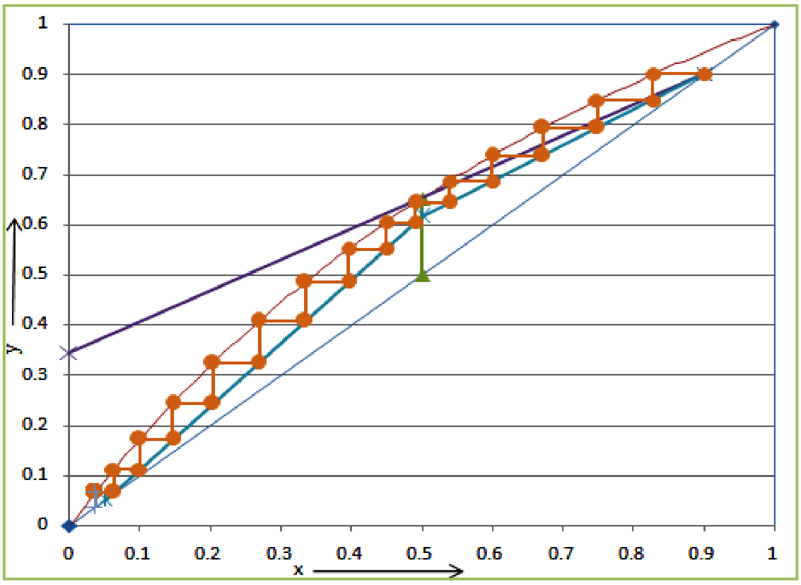


Fig 3- Spreadsheet of McCabe-Thiele diagram for determining the number of stages in the rectifying and stripping sections of a distillation column

Slope of minimum reflux ratio operating line -

Now the minimum reflux must be calculated. This is done by finding the intersection of the q-line (the quality of the liquid) with that of the operating line and the VLE curve. Based on the distillate, this point occurs at:

$$m_{q\text{-line}} = (y_{VLE} – y_F)/(x_{VLE} – x_F)$$

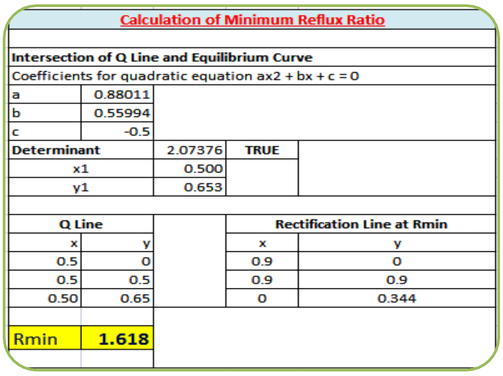
The subscript "F" refers to the feed. All of the above values are known except x_{VLE}, and y_{VLE}.

The cells used for this calculation are shown in Table 6.

For a saturated liquid whose q-line is vertical, a very large slope is calculated (see the upper part of Table 6). The lower part of Table 6 shows the slope of the operating line for minimum reflux:

$$m_{Rmin} = (x_D – y_{VLE})/(x – x_{VLE}) \qquad (15)$$

Table 6- Stripping and rectifying operating lines calculations



Calculation of Minimum Reflux Ratio				
Intersection of Q Line and Equilibrium Curve				
Coefficients for quadratic equation ax2 + bx + c = 0				
a	0.88011			
b	0.55994			
c	-0.5			
Determinant		2.07376	TRUE	
x1		0.500		
y1		0.653		
Q Line			Rectification Line at Rmin	
x	y		x	y
0.5	0		0.9	0
0.5	0.5		0.9	0.9
0.50	0.65		0	0.344
Rmin	1.618			

Optimum operating conditions

Once the minimum reflux conditions are set, m_{Rmin} is multiplied by the predefined optimum reflux multiplier. The optimum reflux ratio, R, is now defined by the slope of the upper or rectifying operating line. To fully define the system, the point of intersection of the operating line and the q-line must be known, after which the slope of the lower (stripping) operating line can be calculated easily. Using the operating line slope, m_R, the following equations are employed to find the intersection of the operating line with the q-line at (xi, yi). Based on the upper or rectifying line the equation is:

$$y_i = m_R(x_i – x_D)/x_F$$

This equation has two unknowns, thus, an expression for xi is formulated from the stripping line:

$$x_i = [(x_F + m_R)/m_{q\text{-line}} – x_F]/(m_R/x_{D*}m_{q\text{-line}} – 1)$$

When the intersection is found, then the slopes of all the operating lines are calculated by simple algebra,. Using the lower and upper operating lines, the previously mentioned algorithm for the Mc-Cabe Thiele diagram is employed to calculate each stage's equilibrium values.

Use of conditional statement -

Throughout all of the calculations, incorporating the upper and lower segmentation lines is accomplished by the using the "if" conditional statement. This statement is crucial in calculating the VLE data for the constant y segment of the calculation. Further, an additional "if" statement is necessary at the transition of the stripping and rectifying lines when calculating beyond the values at the intersections of the lines. When the x value of intersection of the operating lines is passed, the spreadsheet uses the stripping operating line to calculate the y values. This is why the segmentation sheet of Table 3 must determine the segmentation transition value of x, as well as that of y. To find the number of equilibrium stages, note the stage at which the required bottoms conditions are met. For this case, assume that a bottoms x_B value of approximately 0.05 meets the process requirements. The value for Stage 14 is about 0.08, while that for Stage 15 is about 0.05, so there are 15 equilibrium stages. Further calculations are made to find the number of actual stages, the column height, the energy transferred in the reboiler and condenser, and the column diameter (based on the calculated vapor flowrates). These calculations use methods found in standard references, are relatively straightforward, and will only be summarized here.

Column height and flowrates -

The height is simply the number of actual stages multiplied by the tray spacing or packing equivalent height. The flowrates are calculated via mass balances. The equations are taken from Treybal ((4), pp. 402–420). Spreadsheets are easily created to perform all of these calculations and convert the results into different systems of units, when desirable.

Reboiler and condenser duties

Calculations of the energy rates of the reboiler and the condenser are made using latent heats and specific heats (when needed).[7] The calculations are as thus performed piecewise, using each chemical species and its respective latent and specific heats. For example, the bottoms is considered to be made up of 100% Acetic Acid, so its heat duty would be the flowrate of the Acetic Acid vapor rising up from this stage (at 118°C), multiplied by the latent heat of Acetic Acid to create the vapor.

Column diameter -

A method described by Kister ((5), pp. 276–279) determines the upper and lower column diameters. Calculations are based on the flooding velocity, the properties of the liquids and vapors, and the fractional hole area in the trays, among other factors. The calculation is straightforward and is not included here.

VIII. CONCLUSION

By using various mathematical tools in Excel spreadsheet, the numerical solution to a McCabe-Thiele diagram to find the theoretical number of stages for binary and pseudo-binary systems is presented, also the spreadsheet automatically calculates the actual number of stages, reflux ratio and column dimensions and each plate composition. Once, such spreadsheet created, it is very easy to solve another distillation design problems by varying Feed Conditions, Temperature profile and other parameters to give answers quickly.

Nomenclature -

A,B,C = constants for Raoult's law, dimensionless
r_1, r_2, q_1, q_2, a_{12}, a_{21}= constants in Uniquac equation, dimensionless
n = number of data points
P = pressure, Pa
q = quality of liquid
T = temperature, K
x = liquid mole fraction
y = vapor mole fraction

Greek letters:

α = relative volatility
γ = activity coefficient

Subscripts:

1, 2 = component 1 or 2
B = bottoms
D = distillate
F = feed
i = data point
l = mixture
sat = saturated
R = reflux
VLE = at vapor/liquid equilibriu

LITERATURE CITED

[1]. McCabe, W. L., and E. W. Thiele, "Graphical Design of Fractionating Columns," *Ind. Eng. Chem.*, 17, pp. 605–611 (1925).
[2]. Van Winkle, M., "Distillation," McGraw Hill, New York, Toronto (1967).
[3]. Molecular Thermodynamics of Fluid-Phase Equilibria, 3'rd ed., Prentice Hall International Series *by* John M. Prausnitz.
[4]. Perry, R. H., and D. W. Green, eds., "Perry's Chemical Engi- neers' Handbook," 7th ed., McGraw Hill, New York, p. 13-20 (1997).
[5]. Paul M. Mathias, "Visualizing the McCabe Thiele Diagram", Ameriacan Institute of Chemical engineers,CEP, 2009.
[6]. Jake Jevric, Muhammad E. Fayed, "Shortcut Distillation Calculations via Spreadsheets, Ameriacan Institute of Chemical engineers",CEP, 2002.
[7]. Principles of Mass Transfer and Separation Processes, Prentice Hall India Pvt. Limited, Eastern Economy Edition, 2007, *by* Binay K. Dutta.
[8]. Chemical Engineering, Butterworth-Heinemann Publication, Vol. 2, Fifth Edition, 2002, *by* J.M.Coulson and J.R.Richardson.
[9]. Burns, M. A., and J. C. Sung, "Design of Separation Units Using Spreadsheets," *Chem. Eng. Education*, 30, pp. 62–69 (1996).
[10]. Eva Sorensen, "Principles of Binary Sepeartion", Department of Chemical Engineering, UCL, London, UK, Chapetr 4,146-185.
[11]. Treybal, R. E., "Mass Transfer Operations," McGraw Hill, New York (1987).
[12]. Kister, H. Z., "Distillation Design," McGraw-Hill, New York (1992).