Determination of the Flowrates of Vapour and Liquid in a Binary Distillation Column using MS Excel
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Abstract:
The importance of the equilibrium (x-y) curve in the determination of the minimum reflux ratio for the design of a binary distillation column was explained. This study shows the use of MS Excel drawing tools to construct the q-line for the determination of the minimum reflux ratio in the McCabe-Thiele diagram. The feed enters at its bubble point since the q-line is vertical. A careful study reveals that without the determination of the actual reflux ratio, the flow rates of vapour and liquid cannot be evaluated. MS Excel uses the principle of matrix in solving the mass balance equations to obtain the flow rates of vapour and liquid. The following parameters were determined for the binary distillation column: the minimum reflux ratio (0.979), the actual reflux ratio (1.958), the bottom product (1166.67 Kmol/hr), the top product (1833.33 Kmol/hr), the Liquid flow rate at the top section (3589.66 kmol/hr), Liquid flow rate from the bottom section (6589.66 kmol/hr), the vapour flow rate in the column (5422.99 kmol/hr), the vapour mass flow rate (134.24 kg/sec), the liquid mass flow rate (163 kg/sec) and the vapour volumetric flow rate (49.42 m³/sec). Further work will be on the use of other softwares to determine the flowrates of vapour and liquid.

Keywords: Column, determination, distillation, flowrates, liquid, MS Excel.

I. INTRODUCTION
Distillation is a separation process used to separate two or more components into an overhead distillate and bottoms where the bottoms product is liquid, and the distillate may be liquid or a vapor or both [11;12; 13; 14]. Distillation is based on the fact that the vapor of a boiling mixture will be richer in the components that have lower boiling points. There are many types of distillation columns, each one of them is designed to be used in specific kind of separation. Depending on how they are operated they can be classified to: Continuous or Batch distillation columns [1; 2]. Binary distillation is a special distillation process. It is a multistage process for separating a mixture of two components [5; 8; 9]. The separation process requires that (i) a second phase be formed so that both vapor and liquid phases can contact each other on each stage within a separation column, (ii) the components have different volatilities so that they will partition between the two phases to different extents, and (iii) the two phases can be separated by gravity or other mechanical means [16]. A binary distillation column showing the top and bottom stages is shown in Figure 1. Ideally, the more volatile component is separated as vapor and flows out from top. The less volatile component flows out at bottom as liquid. The product for a binary distillation process is a pure component, or technically a purer component. The component can be obtained by collecting the vapor flow or the liquid flow. There are two ways to do distillation calculations by McCabe Thiele method. One is graphical method and other way is by using any other commercial simulation software. The graphical method is by hand and is time consuming. The use of the commercial simulation software though is costly and requires license is the best especially when different mixtures are involved. In this paper, Ms –Excel is used to determine the flowrates of vapour and liquid in a binary distillation column. The McCabe Thiele’s equations are given elsewhere [3; 11; 12; 13; 14; 17; 18; 19].

Figure 1. Binary Distillation Column Showing The Top And Bottom Stages

2. METHODOLOGY

2.1 The Procedure
McCabe and Thiele method uses the equilibrium curve diagram to determine the number of theoretical stages (trays) required to achieve a desired degree of separation. It assumes constant molar overflow and this implies that: (i) molar heats of vaporization of the components are roughly the same; (ii) heat effects are negligible. The information required for the
systematic calculation are the vapour liquid equilibrium (VLE) data, feed condition (temperature, composition), distillate and bottom compositions; and the reflux ratio, which is defined as the ratio of reflux liquid over the distillate product. Figure 1 is usually separated into the top section and bottom section of the binary distillation column. The detail procedures for the McCabe and Thiele Method are shown elsewhere [1; 3; 5; 7; 9; 16; 19].

2.2 The Design problem

Suppose, we are going to design a distillation column to separate benzene-toluene mixture with feed flow rate 3000Kmole/hr, the feed is saturated liquid, the feed has 60% mol fraction of benzene and the over head product has 0.95 mol fraction of benzene and the bottom product contain 0.05 mol fraction of benzene. The system operates in partial reboiler and total condenser modes. The distillation column also operates at atmospheric pressure (p= 1atm) and the operating reflux ratio is 2. The design specifications are shown in table 1. The variables in table 1 that are not found in the table 2. The variables in table 1 that are not found in the study, they calculated the TXY data and plotted the curve (XY) diagram of a binary distillation column has been done and reported elsewhere [19]. In their study, they calculated the TXY data and plotted the equilibrium curve (XY) diagram using hand and excel. The TXY data is presented in table 2 and how the equilibrium curve (X-Y) diagram was plotted with MS Excel is shown in figure 2.

Table:1. Design specifications

<table>
<thead>
<tr>
<th>Feed rate</th>
<th>3000 Kmole/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed composition</td>
<td>60% benzene, 40% toluene</td>
</tr>
<tr>
<td>Column operating pressure</td>
<td>Atmospheric (1atm)</td>
</tr>
<tr>
<td>Column reboiler</td>
<td>Partial</td>
</tr>
<tr>
<td>Column condenser</td>
<td>Total</td>
</tr>
<tr>
<td>Distillate composition, x_d</td>
<td>95% benzene</td>
</tr>
<tr>
<td>Bottom composition, x_b</td>
<td>95% toluene</td>
</tr>
<tr>
<td>Relative volatility of benzene to toluene</td>
<td>2.3</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td>2</td>
</tr>
<tr>
<td>Molecular weight of benzene, MW_b</td>
<td>78.114 kg/kmol</td>
</tr>
<tr>
<td>Molecular weight of toluene, MW_t</td>
<td>92.141 kg/kmol</td>
</tr>
<tr>
<td>Boiling point of benzene</td>
<td>80.1 °C</td>
</tr>
<tr>
<td>Boiling point of toluene</td>
<td>110.6 °C</td>
</tr>
<tr>
<td>Vapour density of benzene</td>
<td>2.77kg/m³</td>
</tr>
<tr>
<td>Vapou density of toluene</td>
<td>876kg/m³</td>
</tr>
<tr>
<td>Plate or tray spacing</td>
<td>0.5m</td>
</tr>
</tbody>
</table>

2.3 Assumptions made during the design

The McCabe-Thiele method of column design is used with the following assumptions inherent in the calculation:
• Constant vapor and liquid flow rates in any given section of the tower.
• The latent heat of evaporation is approximately constant with composition and also does not vary much as we proceed from tray to tray.
• The system is non-foaming and non corrosive, and thus we can use carbon steel rather than stainless steel as our material of construction.

2.4 Design steps

Though our concern in this study is the determination of the actual reflux ratio of a binary distillation Column using Excel, the following steps should be followed in the binary distillation column design [4; 6; 8; 13; 15].

i. Determine the vapor-liquid equilibrium curve (x-y diagram) from Antoine data.

ii. Obtain the physical data of benzene and toluene required for the design.

iii. Calculate the flow rate of various stream through the column.

iv. Calculate the minimum reflux ratio and the minimum number of trays required.

v. Using the physical data and flow rates calculate the reboiler and condenser duties.

vi. Calculate maximum and minimum liquid and vapor flow rates.

vii. To start the iteration, select reasonable plate spacing and using the trial plate spacing calculate the column diameter.

viii. Select a trial plate layout, select down-comer area, active, area and size, weir height and length.

ix. From this data check that the weeping rate is satisfactory.

x. Calculate the plate pressure drop.

xi. Check that the down-comer area backup is acceptable.

xii. If at any stage some of the values are too high or low select new trial values and repeat the iterations above.

2.5 Determination of the Actual reflux ratio of a binary distillation Column using Excel

A detail design calculations of the TXY data and drawing of the equilibrium curve (XY) diagram of a binary distillation column has been done and reported elsewhere [19]. In their study, they calculated the TXY data and plotted the equilibrium curve (X-Y) diagram using hand and excel. The TXY data is presented in table 2 and how the equilibrium curve (X-Y) diagram was plotted with MS Excel is shown in figure 2.

Table 2. Txy data for benzene and toluene (yousuo et al., 2019)

<table>
<thead>
<tr>
<th>Temp. (°C)</th>
<th>$P_b^0$ (mmHg)</th>
<th>$P_t^0$ (mmHg)</th>
<th>$x_b$</th>
<th>$y_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>80.1</td>
<td>760.0</td>
<td>292.2</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>82</td>
<td>805.5</td>
<td>311.9</td>
<td>0.91</td>
<td>0.96</td>
</tr>
<tr>
<td>84</td>
<td>855.7</td>
<td>333.7</td>
<td>0.82</td>
<td>0.91</td>
</tr>
<tr>
<td>86</td>
<td>908.3</td>
<td>356.8</td>
<td>0.73</td>
<td>0.86</td>
</tr>
<tr>
<td>88</td>
<td>963.3</td>
<td>381.1</td>
<td>0.65</td>
<td>0.81</td>
</tr>
<tr>
<td>90</td>
<td>1021.0</td>
<td>406.7</td>
<td>0.58</td>
<td>0.76</td>
</tr>
<tr>
<td>92</td>
<td>1081.3</td>
<td>433.7</td>
<td>0.50</td>
<td>0.70</td>
</tr>
<tr>
<td>94</td>
<td>1144.3</td>
<td>462.1</td>
<td>0.44</td>
<td>0.64</td>
</tr>
<tr>
<td>96</td>
<td>1210.1</td>
<td>492.0</td>
<td>0.37</td>
<td>0.58</td>
</tr>
<tr>
<td>98</td>
<td>1278.8</td>
<td>523.4</td>
<td>0.31</td>
<td>0.51</td>
</tr>
<tr>
<td>100</td>
<td>1350.5</td>
<td>556.3</td>
<td>0.26</td>
<td>0.44</td>
</tr>
<tr>
<td>102</td>
<td>1425.2</td>
<td>590.9</td>
<td>0.20</td>
<td>0.37</td>
</tr>
<tr>
<td>104</td>
<td>1503.1</td>
<td>627.2</td>
<td>0.15</td>
<td>0.29</td>
</tr>
<tr>
<td>106</td>
<td>1584.2</td>
<td>665.2</td>
<td>0.10</td>
<td>0.21</td>
</tr>
<tr>
<td>108</td>
<td>1668.6</td>
<td>704.9</td>
<td>0.06</td>
<td>0.12</td>
</tr>
<tr>
<td>110</td>
<td>1756.4</td>
<td>746.6</td>
<td>0.01</td>
<td>0.03</td>
</tr>
<tr>
<td>110.6</td>
<td>1784.5</td>
<td>760</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
2.6. Determination of the Minimum reflux ratio\( (R_{\text{mm}})\) of a binary distillation column:

To determine the minimum reflux ratio, use the drawing tools of MS Excel to construct the q-line and identify its point of intersection with the equilibrium curve and then draw a line from product composition point on the 45˚diagonal line to this intersection point as shown in figure 3. The slope of the q-line is \(R_{\text{mm}}/(1+R_{\text{mm}})\) and the intercept of the q-line on the y-axis is \(x_{d}/(1+R_{\text{mm}})\). Minimum reflux can be determined from either of these.

This implies that \(x_{d}/(1+R_{\text{mm}}) = 0.48\)
\[
\frac{0.95}{1 + R_{\text{mm}}} = 0.48
\]
\[
(1 + R_{\text{mm}}) = 0.48
\]
\[
R_{\text{mm}} = 0.979
\]

Therefore the minimum reflux ratio is \(0.979\).

2.7. Determination of the actual reflux ratio\( (R_{\text{mm}})\) of a binary distillation column

\[
R = (1.2 \ldots \ldots \ldots 2)R_{\text{mm}}
\]
\[
R = 2R_{\text{mm}} = 2 \times 0.979 = 1.958.
\]

So, the actual reflux ratio is 1.958.

2.8. Determination of the flowrates of vapour and liquid in a binary distillation column

Considering figure 1, the overall balance is given by equation (1)
\[
F = D + B
\]
Where:
\(F\) = feed
\(D\) = Gas or Distillate (top product)
\(B\) = Liquid (bottom product)
\[
3000 = D + B
\]
\[
D = 3000 - B \quad (2)
\]

Considering figure 1 again, the component balance for benzene is given by (3)
\[
F_{B} \cdot F = X_{d} \cdot D + X_{b} \cdot B
\]
Where:
\(F_{B}\) = Mole fraction of benzene in the feed
\(X_{d}\) = Mole fraction of benzene in the distillate
\(X_{b}\) = Mole fraction of benzene in the bottom product

\[
0.6 \cdot 3000 = 0.95 \cdot D + 0.05 \cdot B
\]
\[
1800 = 0.95D + 0.05B \quad (4)
\]

Substitute (2) in (4):
\[
1800 = 0.95(3000 - B) + 0.05B
\]
\[
B = 1166.67 \text{ Kmol/hr}
\]
\[
D = 1833.33 \text{ Kmol/hr}
\]

The value of B and D can easily be calculated with MS Excel as follows.

Using EXCELL

Re-arranging (1) and (3) gives
\[
D + B = F
\]
\[
X_{d} \cdot D + X_{b} \cdot B = F_{B} \cdot F
\]

(5) and (6) gives a 2 by 2 coefficient matrix of the form
\[
A \cdot X = B
\]
Where:
\[
A = \begin{bmatrix} 1 & X_{d} \\ X_{b} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0.95 \\ 0.05 & 1 \end{bmatrix}
\]
\[
B = \begin{bmatrix} F \\ F_{B} \cdot F \end{bmatrix} = \begin{bmatrix} 3000 \\ 1800 \end{bmatrix}
\]
$$X = \begin{bmatrix} D \end{bmatrix} = BA^{-1}$$

In the Excel Microsoft spread sheet (figure 4) or user interface type as follows:

- **X_d** = 0.95
- **X_w** = 0.05

Matrix A

$$\begin{bmatrix} X_d & X_w \end{bmatrix}$$

Microsoft excel can be used to calculate, the determinant of A, inverse of matrix A and $$X = \begin{bmatrix} D \end{bmatrix} = BA^{-1}$$

For determinant of matrix A, the excel syntax used is

**MDet(arrary) and pressing Enter key**

For Inverse of Matrix A, the excel syntax used is

**MINVERSE(array) and pressing Shift, Control and Enter key**

To calculate Matrix X = $[D] = BA^{-1}$

**MMULT(array1,array2) and pressing Shift, Control and Enter Keys at the same time.**

2.8.1. Explanation to figure 4

An array is C8:D9

- An array 1 is C12:D13
- And array 2 is G12:G13

An array is C8:D9

2.8.1. Explanation to figure 4

An array is C12:D13

And array 2 is G12:G13

D = 1833.33 Kmol/hr
B= 1166.67 Kmol/hr
We have determine R from section 2.6 to be 1.958
And so we can determine the flow rates of vapour and liquid through the column

- **The Liquid flow rate the top section**, L=RD = 1.958 X 1833.33 = 3589.66 Kmol/hr.
- **Liquid flow rate from the bottom section**, L' =L+F =RD+F = 1.958 X 1833.33 + 3000 = 6589.66 Kmol/hr.
- **Vapor flow rate in the column**, G=L+D=RD+D=(R+1)D = (1.958 + 1)1833.33 = 5422.99 Kmol/hr.

- **Vapor mass flow rate**, $$V_v = (G) * MW_v$$
  - $$MW_{av} = 0.6 * 78.144 + 0.4 * 92.141 = 89.12 kg/kmol$$
  - $$V_v = (G) * MW_{av} = 5422.99 * 89.12 = 134.24$$
  - **Liquid mass flow rate**, $$L_w = (L) * MW_{av} = 6589 * 89.12 = 587270.49 kg/hr = 163 kg/sec$$
  - **Vapor volumetric flow rate**, $$Q_v = \frac{V_v}{\rho_v} = \frac{134.24}{2.716} = 49.42 m^3/sec$$

3. DISCUSSION AND CONCLUSION

This study shows the use of MS Excel drawing tools to construct the q-line for the determination of the minimum reflux ratio in the McCabe-Thiele diagram. The feed enters at its bubble point since the q-line is vertical. A careful study reveals that without the determination of the actual reflux ratio, the flow rates of vapour and liquid cannot be evaluated. MS Excel uses the principle of matrix in solving the mass balance equations. MS Excel has the ability to store values when commanded and a change in one value will have a corresponding change in the others, depending on the equations and relationship used, hence new mass balance equations can be solved with ease. The following parameters were determined for the binary distillation column: the minimum reflux ratio (0.979), the actual reflux ratio (1.958), the bottom product (1166.67 Kmol/hr), the top product (1833.33 Kmol/hr), the Liquid flow rate at the top section (3589.66 Kmol/hr), Liquid flow rate from the bottom section (6589.66 Kmol/hr), the vapour flow rate in the column (5422.99 Kmol/hr), the vapour mass flow rate (134.24 kg/sec), the liquid mass flow rate (163 kg/sec) and the vapour volumetric flow rate (49.42 m³/sec). Further work will be on the use of other softwares to determine the flowrates of vapour and liquid.

4. REFERENCES


[5]. Jing Yan (2012). Robust Design of the parameters for a Distillation System, a Thesis Submitted to the graduate faculty of north Caroline State University in Partial Fulfillment of the Requirements for the Degree of Masters of Science in Industrial Engineering.


