MODULE 5: DISTILLATION

LECTURE NO. 4

5.2.2.3. Analysis of binary distillation in tray towers: McCabe-Thiele Method

McCabe and Thiele (1925) developed a graphical method to determine the theoretical number of stages required to effect the separation of a binary mixture (McCabe and Smith, 1976). This 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) molal heats of vaporization of the components are roughly the same; (ii) heat effects are negligible. The information required for the systematic calculation are the 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. For example, a column is to be designed for the separation of a binary mixture as shown in Figure 5.11.
Figure 5.11: Schematic of column for separation of binary mixture

The feed has a concentration of $x_F$ (mole fraction) of the more volatile component, and a distillate having a concentration of $x_D$ of the more volatile component and a bottoms having a concentration of $x_B$ is desired. In its essence, the method involves the plotting on the equilibrium diagram three straight lines: the rectifying section operating line (ROL), the feed line (also known as the q-line) and the stripping section operating line (SOL). An important parameter in the analysis of continuous distillation is the Reflux Ratio, defined as the quantity of liquid returned to the distillation column over the quantity of liquid withdrawn as product from the column, i.e. $R = \frac{L}{D}$. The reflux ratio $R$ is important because the concentration of the more volatile component in the distillate (in mole fraction $x_D$) can be changed by changing the value of $R$. The steps to be followed to determine the number of theoretical stages by McCabe-Thiele Method:

- Determination of the Rectifying section operating line (ROL).
- Determination the feed condition (q).
- Determination of the feed section operating line (q-line).
- Determination of required reflux ratio (R).
- Determination of the stripping section operating line (SOL).
• Determination of number of theoretical stage.

**Determination of the Rectifying section operating line (ROL)**

Consider the rectifying section as shown in the Figure 5.12. Material balance can be written around the envelope shown in Figure 5.12:

Overall or total balance:

\[ V_{n+1} = L_n + D \]  

(5.13)

Component balance for more volatile component:

\[ V_{n+1} y_{n+1} = L_n x_n + D x_D \]  

(5.14)

From Equations (4.13) and (4.14), it can be written as

\[ (L_n + D) y_{n+1} = L_n x_n + D x_D \]  

(5.15)

Consider the constant molal flow in the column, and then one can write: \( L_1 = L_2 = \ldots \) \( L_{n-1} = L_n = L_{n+1} = L = \) constant and \( V_1 = V_2 = \ldots \) \( V_{n-1} = V_n = V_{n+1} = V = \) constant. Thus, the Equation (5.15) becomes:

\[ (L + D) y_{n+1} = L x_n + D x_D \]  

(5.16)
After rearranging, one gets from Equation (5.16) as:

\[ y_{n+1} = \left( \frac{L}{L+D} \right)x_n + \left( \frac{D}{L+D} \right)x_D \]  

(5.17)

Introducing reflux ratio defined as: \( R = \frac{L}{D} \), the Equation (5.17) can be expressed as:

\[ y_{n+1} = \left( \frac{R}{R+1} \right)x_n + \left( \frac{1}{R+1} \right)x_D \]  

(5.18)

The Equation (5.18) is the rectifying section operating line (ROL) Equation having slope \( \frac{R}{(R+1)} \) and intercept, \( \frac{x_D}{(R+1)} \) as shown in Figure 5.13. If \( x_n = x_D \), then \( y_{n+1} = x_D \), the operating line passed through the point \( (x_D, x_D) \) on the 45° diagonal line. When the reflux ratio \( R \) changed, the ROL will change. Generally the
rectifying operating line is expressed without subscript of n or n+1. Without subscript the ROL is expresses as:

\[ y = \left( \frac{R}{R+1} \right) x + \left( \frac{1}{R+1} \right) x_D \]  

(5.19)

**Figure 5.13: Representation of the rectifying operating line**

**Determination the feed condition \((q)\):**

The feed enters the distillation column may consists of liquid, vapor or a mixture of both. Some portions of the feed go as the liquid and vapor stream to the rectifying and stripping sections. The moles of liquid flow in the stripping section that result from the introduction of each mole of feed, denoted as ‘q’. The limitations of the q-value as per feed conditions are shown in Table 5.3.
Table 5.3: Limitations of q-value as per feed conditions

<table>
<thead>
<tr>
<th>Feed condition</th>
<th>Limit of q-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>cold feed (below bubble point)</td>
<td>q &gt; 1</td>
</tr>
<tr>
<td>feed at bubble point (saturated liquid)</td>
<td>q = 1</td>
</tr>
<tr>
<td>feed as partially vaporized</td>
<td>0 &lt; q &lt; 1</td>
</tr>
<tr>
<td>feed at dew point (saturated vapor)</td>
<td>q = 0</td>
</tr>
<tr>
<td>feed as superheated vapor</td>
<td>q &lt; 0</td>
</tr>
<tr>
<td>feed is a mixture of liquid and vapor</td>
<td>q is the fraction of the feed that is liquid</td>
</tr>
</tbody>
</table>

**Calculation of q-value**

*When feed is partially vaporized:*

Other than saturated liquid (q = 1) and saturated vapor (q = 0), the feed condition is uncertain. In that case one must calculate the value of q. The q-value can be obtained from enthalpy balance around the feed plate. By enthalpy balance one can obtain the q-value from the following form of Equation:

$$ q = \frac{H_v - H_L}{H_v - H_L} $$

(5.20)

where $H_F$, $H_V$, and $H_L$ are enthalpies of feed, vapor, and liquid respectively which can be obtained from enthalpy-concentration diagram for the mixture.

*When feed is cold liquid or superheated vapor:*

q can be alternatively defined as the heat required to convert 1 mole of feed from its entering condition to a saturated vapor; divided by the molal latent heat of vaporization. Based on this definition, one can calculate the q-value from the following Equations for the case whereby $q > 1$ (cold liquid feed) and $q < 0$ (superheated vapor feed) as:
For cold liquid feed:

\[
q = \frac{C_{p,L}(T_{bp} - T_F) + \lambda}{\lambda}
\]  
(5.21)

For superheated vapor feed:

\[
q = \frac{C_{p,V}(T_{dp} - T_F)}{\lambda}
\]  
(5.22)

where \( T_{bp} \) is the bubble point, \( \lambda \) is the latent heat of vaporization and \( T_{dp} \) is the dew point of the feed respectively.

**Determination of the feed section operating line (q-line):**

Consider the section of the distillation column (as shown in Figure 5.11) at the tray (called feed tray) where the feed is introduced. In the feed tray the feed is introduced at \( F \) moles/hr with liquid of \( q \) fraction of feed and vapor of \( 1-f \) fraction of feed as shown in Figure 5.14. Overall material balance around the feed tray:

\[
L' = L + qF \quad \text{and} \quad V = V' + (1-q)F
\]  
(5.23)

Component balances for the more volatile component in the rectifying and stripping sections are:

For rectifying section:

\[
V_y = L_x + D_{x_D}
\]  
(5.24)

For stripping section:

\[
V'_{y} = L'_{x} - B_{x_B}
\]  
(5.25)

At the feed point where the two operating lines (Equations (5.24) and (5.25) intersect can be written as:
\[(V - V')y = (L - L')x + Dx_D + Bx_B \quad (5.26)\]

Substituting \(L - L'\) and \(V - V'\) from Equations (5.23) and (5.24) into Equation (5.26) and with Equation (5.27) one can get the q-line Equation after rearranging as:

\[y = -\left(\frac{q}{1-q}\right)x + \left(\frac{1}{1-q}\right)x_F \quad (5.28)\]

For a given feed condition, \(x_F\) and \(q\) are fixed, therefore the q-line is a straight line with slope \(-q / (1-q)\) and intercept \(x_F/(1-q)\). If \(x = x_F\), then from Equation
(5.28) \( y = x_F \). At this condition the \( q \)-line passes through the point \((x_F, x_F)\) on the 45° diagonal. Different values of \( q \) will result in different slope of the \( q \)-line. Different \( q \)-lines for different feed conditions are shown in Figure 5.15.