

## Appendix II – H. McCabe-Thiele Analysis

### 1. *Introduction and Assumptions*

When designing a distillation column, it is useful for the engineer to know the ideal number of stages for the column and the optimal location for the feed stream inlet. The McCabe-Thiele method provides this information by means of graphical techniques to determine the number of ideal stages required in the column. Before beginning to use this method, the engineer must know certain characteristics of the process, namely, the compositions and molar flow rates of the feed, distillate, and bottoms lines.

The McCabe-Thiele method is based upon several assumptions that serve to simplify the process. The two components are considered to have equal molar heats of vaporization and negligible heats of mixing. The assumption of equimolar overflow through the tower means that at each point in the distillation column, the molar flow rate of liquid traveling down the column is equal to the molar flow rate of vapor moving up inside the column. The method assumes that the process is adiabatic, is operated at a constant pressure, and has reached steady-state. Finally, the feed stream is assumed to mix with the feed stage before any separation takes place. While this is an idealized situation, the method nonetheless provides information that is useful to the engineer.

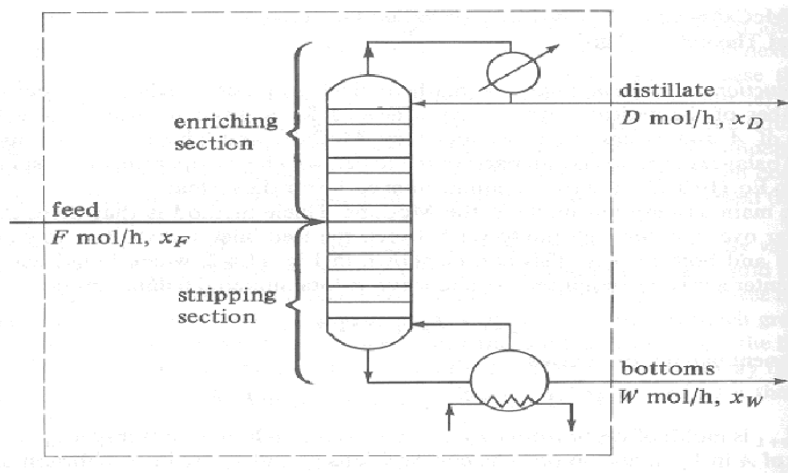
Before proceeding, two conventions used throughout this report should be pointed out. The plates in a distillation column are numbered from the top downward, so that the top plate is designated as 1, and so on. Also, when expressing the compositions of the streams, all compositions are in terms of the mole fraction of the more volatile component.

The technique developed by McCabe and Thiele makes use of an  $xy$  plot in which the mole fraction of the more volatile component in the liquid ( $x$ ) is designated as the abscissa and the mole fraction of this component in the vapor phase ( $y$ ) is designated as the ordinate. The vapor-liquid equilibrium curve is plotted on these axes along with the line  $y = x$ , two operating curves, and a feed curve, which will be described in detail in the sections that follow.

## 2. *The Distillation Column*

A distillation column can be divided into two sections (see Figure 1): the region above the feed line, called the enriching or rectifying section, and the section below the feed line, termed the stripping section.

**Figure 1: Sections of the Distillation Column**



The molar flow rates are termed  $F$ ,  $D$ , and  $W$  for feed, distillate, and bottoms, and the respective mole fractions of the more volatile component are  $x_F$ ,  $x_D$ , and  $x_W$ . All of these quantities are assumed to be constant.

A material balance for the entire column yields the following:

$$F = D + W \quad (1)$$

A material balance on the more volatile component yields:

$$x_F F = x_D D + x_W W \quad (2)$$

Similar material balances can be performed on the enriching and stripping sections of the distillation column.

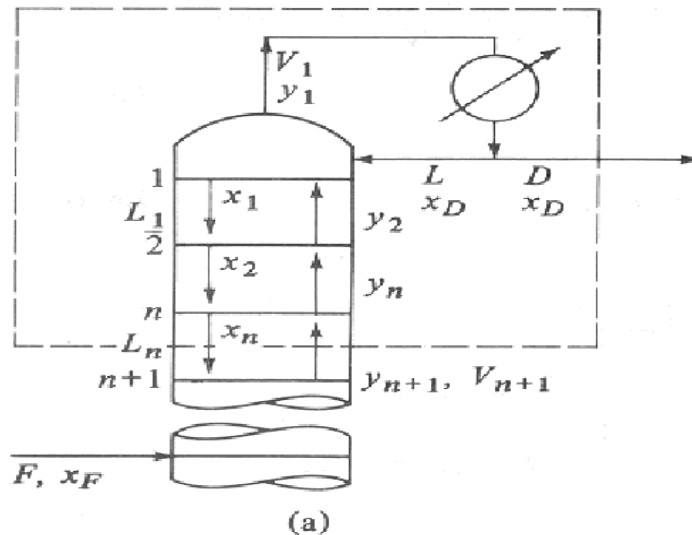
The reflux ratio is defined as the ratio of the liquid to distillate molar flow rate.

$$R = \frac{L_n}{D} \quad (3)$$

### 3. *The Enriching and Stripping Sections*

A material balance can be carried out in the rectifying section by focusing on one plate. If a given plate is labeled  $n$ , the plate below it is referred to as  $n+1$ , and so on. When vapor exits the top of the enriching section and passes to the condenser, the composition does not change, and in Figure 2,  $y_1 = x_D$ .

**Figure 2: Schematic of Enriching Section**



A total material balance on the enriching section yields:

$$V_{n+1} = L_n + D \quad (4)$$

In equation (4),  $V_{n+1}$  denotes the vapor flowing from plate  $n+1$  to plate  $n$ ,  $L_n$  indicates the liquid descending from plate  $n$ , and  $D$  is the distillate product. A material balance on component A yields:

$$y_{n+1}V_{n+1} = x_nL_n + x_D D \quad (5)$$

Solving this equation for  $y_{n+1}$  provides the operating line for the enriching section.

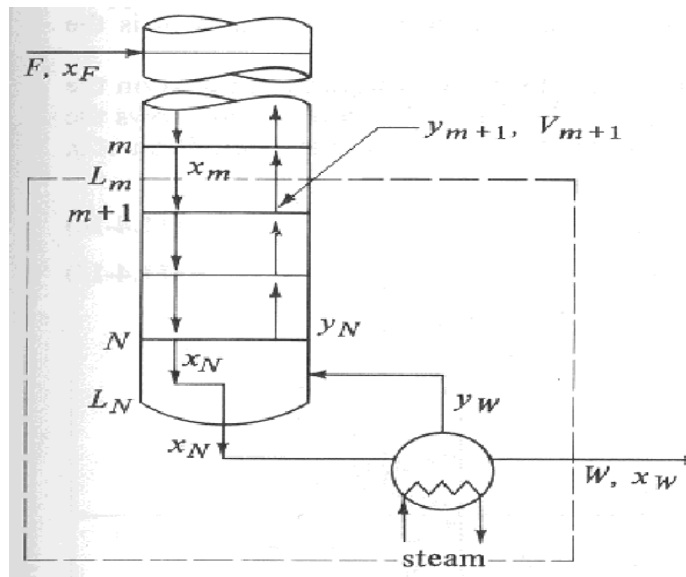
$$y_{n+1} = \frac{x_nL_n + x_D D}{V_{n+1}} = \frac{L_n}{V_{n+1}}x_n + \frac{x_D D}{V_{n+1}} \quad (6)$$

This line can be plotted on the  $xy$  graph: the operating line intersects the line  $y = x$  at the point  $x = x_D$ , and the slope of the line is  $L_n/V_{n+1}$ . The operating line can also be rewritten in terms of the reflux ratio.

$$y_{n+1} = \frac{R}{R+1}x_n + \frac{x_D}{R+1} \quad (7)$$

In the stripping section, a material balance is carried out by focusing on one plate. In this section of the column, plates are labeled using the letter  $m$  (Figure 3).

**Figure 3: Schematic of Stripping Section**



The overall material balance for the stripping section of the distillation column is

$$L_m = V_{m+1} + W \quad (8)$$

A balance can also be performed on component A.

$$y_{m+1}V_{m+1} = x_mL_m - x_WW \quad (9)$$

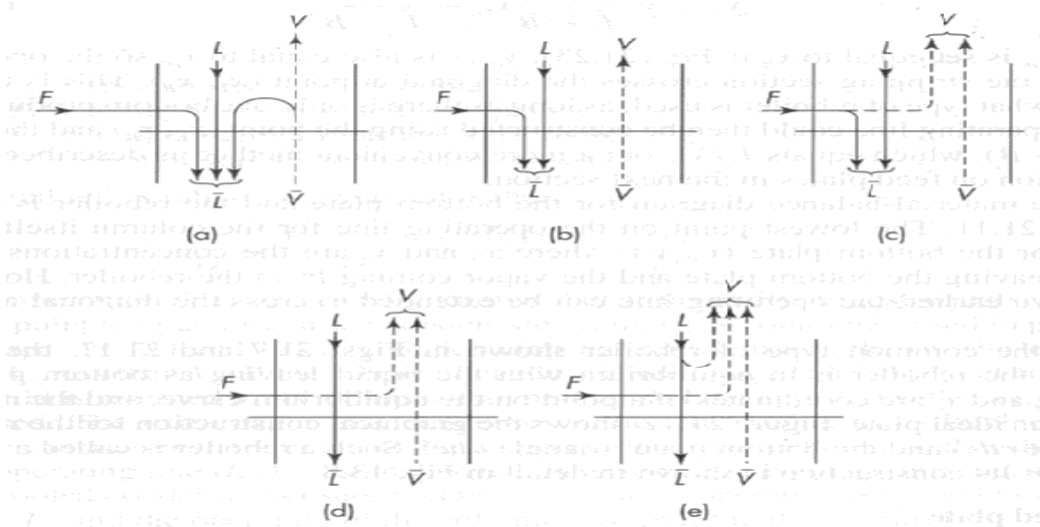
Rearranging the above equation in terms of  $y_{m+1}$  yields the operating curve for the stripping section.

$$y_{m+1} = \frac{x_mL_m - x_WW}{V_{m+1}} = \frac{L_m}{V_{m+1}}x_m - \frac{x_WW}{V_{m+1}} \quad (10)$$

#### 4. The $q$ Factor

The state of the feed to the distillation column is an important parameter for the engineer to know as it is used to determine the equation for the feed line. The following diagram illustrates the behavior of the feed stream as it enters the column.

**Figure 4: Flow Through Feed Plate for Various Feed Conditions:** (a) feed cold liquid; (b) feed saturated liquid; (c) feed partially vaporized; (d) feed saturated vapor; (e) feed superheated vapor.



In Figure 4a, the feed enters as liquid below the bubble point, causing all of the feed to flow downward and also condensing some of the vapor stream. This increases the

flow rate of liquid in the stripping section and decreases the flow rate of vapor to the rectifying section. If the feed is saturated liquid at the bubble point, as in Figure 4b, the feed flows downward. A feed stream that is partially vaporized, Figure 4c, will have liquid that will flow downward and vapor that will flow upward in the column. Figure 4d shows a feed line that is saturated vapor, and all of the feed joins the vapor flow. Finally, in Figure 4e, the feed is superheated vapor, and not only does the entire feed stream flow up the column, but it also vaporizes some of the liquid stream.

The state of the feed stream can be characterized by the  $q$  factor, which is defined as the number of moles of liquid flow in the stripping section resulting from the entrance of one mole of feed into the column. The state of the feed is related to  $q$  as follows:

**Table 1: The  $q$  Factor for the Feed Stream**

State of Feed Stream	Value of $q$
Cold liquid feed	$q > 1$
Saturated liquid at the bubble point	$q = 1$
Partially vaporized feed	$0 < q < 1$
Saturated vapor at the dew point	$q = 0$
Superheated vapor	$q < 0$

The  $q$  factor must be calculated for feed that is cold liquid, partially vaporized, or superheated vapor. For the liquid feed below the bubble point temperature,  $q$  can be calculated as follows,

$$q = 1 + \frac{c_{p,L}(T_b - T_F)}{\Delta H_v} \quad (11)$$

where  $c_{p,L}$  is the specific heat of the liquid,  $T_b$  is the bubble point temperature,  $T_F$  is the temperature of the feed stream, and  $\Delta H_v$  is the heat of vaporization.

For feed that is a mixture of liquid and vapor,  $q$  represents the fraction that is in the liquid phase. This type of feed can result from a flash operation, in which case,

$$q = 1 - f \quad (12)$$

where  $f$  is the fraction of the original feed stream that vaporized in the flash operation.

Feed that is composed entirely of superheated vapor has a  $q$  factor that is defined by the following expression,

$$q = -\frac{c_{p,V}(T_F - T_d)}{\Delta H_v} \quad (13)$$

where  $c_{p,V}$  is the specific heat of the vapor and  $T_d$  is the dew point temperature.

Alternately, the  $q$  factor can be calculated from the following equation.

$$q = \frac{H_V - H_F}{H_V - H_L} \quad (14)$$

In the preceding equation,  $H_V$ ,  $H_L$ , and  $H_F$  represent the enthalpies of the feed stream at the dew point, bubble point, and feed temperature, respectively. All of the enthalpies share the same units, i.e. kJ/mol.

## 5. *The Feed Line*

The equation for the feed line can be obtained from material balances and the  $q$  factor. Remembering that the subscript  $n$  denotes flow in the rectifying section and the subscript  $m$  denotes flow in the stripping section, the flow rates just above and below the feed line can be described as follows.

$$L_m = L_n + qF \Rightarrow L_m - L_n = qF \quad (15)$$

$$V_n = V_m + (1 - q)F \Rightarrow V_m - V_n = -(1 - q)F \quad (16)$$

Equations (6) and (10), the material balances in the rectifying and stripping sections, respectively, can be generalized without the plate subscripts. At the point where these two sections intersect,  $y_n = y_m \equiv y$  and  $x_n = x_m \equiv x$ .

$$yV_n = xL_n + x_D D \quad (17)$$

$$yV_m = xL_m - x_B B \quad (18)$$

Subtracting the Equation (17) from Equation (18) yields:

$$y(V_m - V_n) = x(L_m - L_n) - (x_D D + x_B B) \quad (19)$$

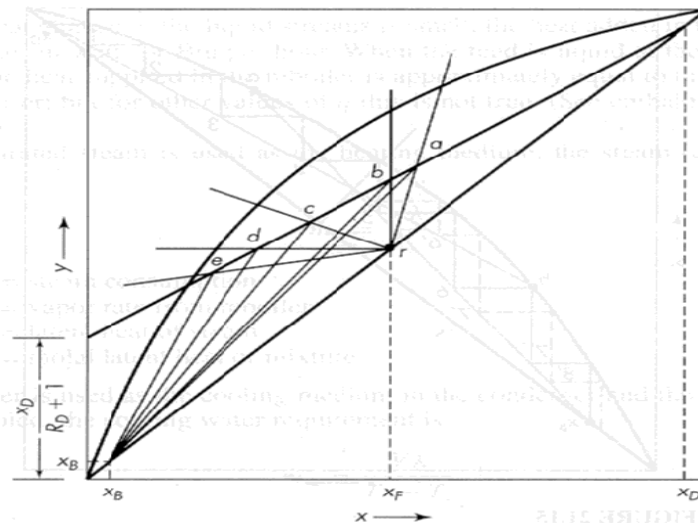
Finally, substituting Equations (2), (15) and (16) into this equation produces the feed line equation.

$$y = -\frac{q}{1-q}x + \frac{x_F}{1-q} \quad (20)$$

## 6. Plotting the Operating Lines

The rectifying section operating line can be graphed by plotting the point  $(x_D, x_D)$  and the y-intercept,  $(0, x_D D/V)$  and connecting the two points. Next, the feed line is plotted, which crosses the line  $y = x$  at the point  $(x_F, y_F = x_F)$ . The slope of the feed line depends on the value of  $q$ , and Figure 5 illustrates the feed lines for each  $q$  value that corresponds to the different states of the feed stream.

**Figure 5: Effect of State of Feed on Feed Line:** *ra*, feed cold liquid; *rb*, feed saturated liquid; *rc*, feed partially vaporized; *rd*, feed saturated vapor; *re*, feed superheated vapor.





The feed line will intersect the operating line for the enriching section of the distillation column, and the operating line for the stripping section also passes through this point. The stripping section operating line can be plotted by connecting this point of intersection with the point  $(x_B, y_W = x_W)$ .

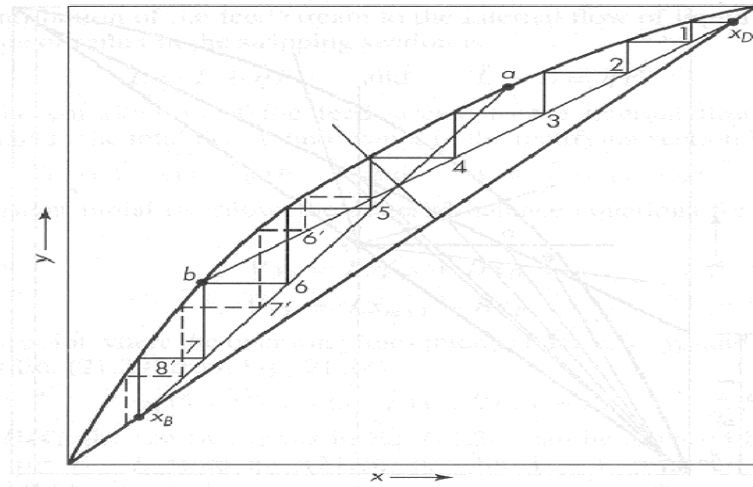
Once the graph has been completed, all that remains is to determine the number of ideal steps. This can be accomplished by starting either at the point  $(x_W, y_W = x_W)$  or  $(x_D, y_D = x_D)$ . Starting at  $(x_D, y_D = x_D)$ , a horizontal line is drawn to the equilibrium line, at which point a vertical line is drawn back down to the operating line for the rectifying section. This process continues until the feed line is reached, at which point the vertical lines are drawn to the operating line for the stripping section. This step-by-step process is continued until the point  $(x_W, y_W = x_W)$  is either reached exactly or passed.

## 7. *Column Performance*

When analyzing the performance of a real column, the location of the feed stream inlet can seriously affect the column performance. Feeding on too low a plate increases the number of plates required in the rectifying section. These plates, as a result, do little separation. Feeding too high in the column leads to similar consequences.

The optimum feed location is found by plotting the operating lines with the vapor-liquid equilibrium line. The optimum feed plate is always represented by the triangle that has one corner on the rectifying line and one corner on the stripping line. At the optimum position, the triangle representing the feed plate straddles the intersection of the operating lines. This is shown graphically in Figure 6.

**Figure 6: Optimum Feed Plate Location**



Upon examination of Figure 6, one can see that the optimum feed plate straddles the intersection of the rectifying and stripping operating lines and is located at plate 5. When the stages are counted off, as soon as the point of intersection of the two operating lines and the feed line is reached, the next operating line should be used in the step-by-step process. In Figure 6, the dashed line represents a process in which the operating line was not switched immediately following the point of intersection, and this error resulted in the need for more plates.

#### **8. *Alternate Method of Performing McCabe-Thiele Analysis***

The previously described method required a knowledge of feed, distillate, and bottoms flow rates and compositions. Alternately, the McCabe-Thiele process can be carried out by using the compositions of the three streams and the reflux ratio. First, the enriching section line is plotted based from reflux ratio using Equation (3) and the feed line is plotted. Next, the point  $(x_W, y_W = x_W)$  is plotted and connected to the point where enriching and feed lines intersect to obtain the operating line for the stripping section. The

number of stages can now be counted as before. This method is useful if the engineer knows the desired reflux ratio for the column rather than the actual flow rates for each stream.

### **9. *Minimum Reflux Ratio***

Before operating a distillation column, it is essential to have an idea of the operating conditions to use to achieve the desired separation. A crucial piece of information to have is the minimum reflux ratio. This is a theoretical minimum that would require an infinite number of stages; therefore, the actual reflux ratio must always be kept above this number.

On a McCabe-Thiele plot, the conditions for the minimum reflux ratio occur when the operating lines for the enriching and stripping sections, the feed line, and the equilibrium curve all intersect at a point known as the pinch point. To obtain this plot, the equilibrium data and the feed line are plotted as usual. The operating line for the enriching section is plotted by connecting the point  $(x_D, y_D = x_D)$  to the pinch point. The minimum reflux ratio can be calculated from the slope of the enriching section operating line (see Equation (7)).

### **10. *The McCabe-Thiele Operating Problem: Estimating Distillate and Bottoms Flow Rates and Compositions***

Up to this point, the use of the McCabe-Thiele method has been restricted to design calculations to determine the number of ideal stages. The method can also be employed to solve the operating problem of estimating the distillate and bottoms flow

rates and compositions for a given column with a set number of stages. The SuperTeam from the previous year developed an approach to solving the operating problem, which is outlined in this section.

The first step in solving the operating problem is to estimate the vaporization rate,  $V_{pred}$ .

$$V_{pred} = \frac{P_R}{\Delta H_{v,ethanol}} \quad (21)$$

To approximate the vaporization rate, the power supplied to the reboiler,  $P_R$ , is divided by the heat of vaporization of the lighter component, ethanol. These two values must be in corresponding units; for example, if the power is given in J/s, the heat of vaporization would be used in units of J/mol to obtain  $V_{pred}$  in units of mol/s.

The power supplied to the reboiler can be calculated using the current,  $I$ , and voltage,  $V_R$ , supplied to the reboiler.

$$P_R = IV_R \quad (22)$$

For current in units of Amperes, A and voltage in units of Volts, V, the resulting value for the power would be in units of Watts, W.

The next step combines the overall material balance on the enriching section, equation (4), with the definition of the reflux ratio, equation (3), in order to obtain an estimate for the liquid flow rate,  $L_{pred}$ .

$$L_{pred} = V_{pred} \left( \frac{R}{R+1} \right) \quad (23)$$

The predicted value for the liquid flow rate is then used to estimate the distillate flow rate,  $D$ . The definition of the reflux ratio is rearranged to provide the following equation:

$$D_{pred} = \frac{L_{pred}}{R} \quad (24)$$

The predicted distillate flow rate can be used in the overall material balance over the entire distillation column, equation (1), to obtain an approximate value for the bottoms flow rate,  $W$ .

$$W_{pred} = F - D_{pred} \quad (1)$$

Only the compositions of the bottoms and distillate streams remain to be calculated. A trial and error procedure is now adopted to arrive at these values. Using the component material balance for the entire column,

$$x_F F = x_D D + x_W W \quad (2)$$

a guess is made for one composition, and the other is calculated using the above equation. The data is then plotted as usual on an  $xy$  plot, and the number of ideal stages are counted. If the number of ideal stages equals the actual number of stages in the column, the process is finished. If the number of ideal and actual stages do not equal, a new guess is made for one composition, the other composition is calculated, the data is plotted and the stages counted, and the process continues until the actual number of stages is reached.

### **11. Example Calculation of the $q$ Factor for the Laboratory Experiment**

The actual value for the  $q$  factor can be calculated using either equation (11) or equation (14). The  $q$  factor will first be computed using equation (11), which applies to liquid feed below the bubble point temperature.

$$q = 1 + \frac{c_{p,L}(T_b - T_F)}{\Delta H_v} \quad (11)$$

The specific heat, bubble point temperature, and heat of vaporization of the feed stream must first be determined. This can be accomplished in two ways – by taking a weighted average of the pure component properties or by using the properties obtained from a ChemCAD simulation. The calculation presented here makes use of the second method. For the following calculations, the feed is considered to be 30 mol% ethanol and 70 mol% propanol, with a temperature of 25 °C and a pressure of 1 atm.

The distillation column was modeled in ChemCAD, which produced values for the required properties of the feed stream. The bubble point temperature was obtained from a TPXY diagram, and the heat of vaporization was evaluated at the bubble point temperature. The heat capacity was evaluated at the average temperature between the bubble point and feed temperature,  $(90+25)/2 = 57.5$  °C.

$$T_b = 90.01 \text{ °C} = 363.16 \text{ K}$$

$$c_{p,L} = 2.7327 \text{ kJ/kg}\cdot\text{K}$$

$$\Delta H_v = 731.9 \text{ kJ/kg}$$

The  $q$  factor can be calculated directly from these values:

$$q = 1 + \frac{c_{p,L}(T_b - T_F)}{\Delta H_v} = 1 + \frac{2.7327(363.16 - 298.15)}{731.9} = 1.24$$

The slope of the feed line is  $-q / (1-q)$ , which equals 5.17.

A second method for calculating the  $q$  factor employs equation (14), which is written in terms of enthalpies.

$$q = \frac{H_V - H_F}{H_V - H_L} \quad (14)$$

Once again, a ChemCAD simulation can be run to determine the enthalpies of the feed mixture at the bubble point temperature, dew point temperature, and feed conditions. A

TPXY diagram was generated to determine the dew point temperature of the feed. The following results were obtained:

$$T_d = 92.79 \text{ }^\circ\text{C}$$

$$H_V = -243.84 \text{ kJ/mol}$$

$$H_L = -285.04 \text{ kJ/mol}$$

$$H_F = -295.04 \text{ kJ/mol}$$

$$q = \frac{H_V - H_F}{H_V - H_L} = \frac{-243.84 + 295.04}{-243.84 + 285.04} = 1.24$$

This method produces a value for slope of the feed line,  $-q / (1-q)$ , of 5.17.

The two techniques that were employed produced identical results for the  $q$  factor to three significant figures. Thus, either technique can be used to obtain the  $q$  factor for the feed stream to a distillation column.