Visualizing the McCabe-Thiele Diagram

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More than 80 years ago, McCabe and Thiele developed a creative graphical solution technique based on Lewis’s assumption of constant molal overflow (CMO) for the rational design of distillation columns (1). The McCabe-Thiele diagram enabled decades of effective design and operational analysis of distillation columns, and has been used to teach several generations of chemical engineers to design and troubleshoot distillation and other cascaded processes.

Simplified methods such as McCabe-Thiele are rarely used today for detailed design. Modern tools are based on rigorous solution of the equations governing cascaded separations, and properly deal with multicomponent systems, heat effects, chemical reactions and mass-transfer limitations (2). Commercially available software enables simulation of entire chemical plants for the purposes of design, optimization and control — but it is important to ensure the discriminating and competent use of these sophisticated tools. The McCabe-Thiele visual approach provides a powerful way to attain this judgment and competency.

Software applications based on rigorous calculations do not explain how distillation really works and how the numerous process variables interact to yield a distillation column that is energy efficient, stable, and produces products with the desired purities. If the design engineer specifies an impossible set of inputs, even the best commercial software either crashes or returns vague and unhelpful messages (e.g., “Tray j dried up”). Engineers who have only performed simulations resort to arbitrary and frantic changes in input variables to obtain a simulation with a feasible specification. In addition, rigorous, computerized calculations do not reveal design problems such as composition pinches and unforgiving composition profiles (i.e., a steep peak in the composition profile of one or more components in multicomponent distillation) — until they are converged. For these reasons, textbooks on staged separations stress the visual approach and present the McCabe-Thiele diagram as an essential tool for understanding and analyzing cascaded operations. Experienced process engineers often use McCabe-Thiele diagrams to understand or help debug simulation results (3). Yet some consider graphical techniques tools of the past, and as a result, the distillation column has become a black box and engineers’ understanding of distillation has suffered (4).

Even though the construction of McCabe-Thiele diagrams is straightforward, it is a tedious and error-prone process. Hence, engineers rarely study the large number of cases needed to understand the interactions of the many process variables. This article introduces a spreadsheet-based approach that readily produces McCabe-Thiele diagrams for binary systems so that the interacting effect of process variables can be visualized easily and interactively; the Excel file is provided as a supplement to the online version of this article (www.aiche.org/cep). Because it is based on the widely available Excel software and uses standard techniques, this method is a useful advance over existing software tools that enable visualization of the McCabe-Thiele diagram.

Excel spreadsheets are increasingly used in chemical engineering education and industrial practice (5). This article demonstrates how Excel may be used for chemical engineering computation and visualization. Through the example presented in the sidebar, the article also demonstrates how the McCabe-Thiele method, and, in particular, the spreadsheet application introduced here, answers typical design questions.
The approach

As far as possible, this application uses Excel’s standard capabilities. The exception is a function to perform data interpolation, called Interp, which was developed using Visual Basic for Applications (VBA) and is provided as part of the online version of the article. This function is used, for example, to interpolate vapor-pressure and x-y equilibrium data. This feature enables the spreadsheet application to accept x-y data from any source, including experimental data, calculated values derived from a thermodynamic model, or values from commercial software.

Figure 1 is a schematic diagram of a distillation column with a total condenser and a partial reboiler. The partial reboiler is an equilibrium stage, but the total condenser is not. The stages are counted from the top down, with stage 1 at the top of the column where the reflux enters. Accordingly to the CMO approximation, each stage is at phase equilibrium, and the vapor and liquid flows are constant in both the rectifying section (above the feed tray) and the stripping section (feed tray and below). Following the usual practice, the compositions refer to the more-volatile component.

The relationships between the reflux ratio \( R = L/D \) and the liquid-to-vapor flow ratio \( L/V \) are:

\[
  \frac{L}{V} = \frac{R}{1+R} \tag{2}
\]

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\[
  \frac{L}{V} = \frac{R}{1+R} \tag{2}
\]

Analogous to Eq. 1, the operating line for the stripping section is:

\[
  y_{j+1} = \frac{L}{V} x_j + \left( \frac{L}{V} - 1 \right) x_B \tag{3}
\]

The feed line, or “q-line,” starts from a point on the \( x = y \) diagonal line where \( x = x_F \) and has a slope based on \( q \) or the liquid fraction of the feed. In the distillation literature, \( q \) is usually referred to as the thermal state of the feed. Note that \( q \) can be less than zero (superheated vapor) or greater than unity (subcooled liquid). The slope of the q-line is \( q/(q - 1) \).

The construction of the two operating lines and the q-line is performed in Excel as follows:

1. The rectifying-section operating line is drawn using Eqs. 1 and 2 and the specified values of \( x_D \) and \( R \).

Example: The Problem Statement

An existing distillation column consists of a total condenser and 10 equilibrium stages, with the feed inlet on the fifth stage from the top. The 10 equilibrium stages include a partial reboiler. The column needs to be reused to separate an acetone-ethanol binary mixture at a pressure of 1 atm. The feed is 20% vaporized and contains 50 kmol/h acetone and 50 kmol/h ethanol. The desired distillate and bottoms compositions of acetone are 90 mole% and 3 mole%, respectively. Vapor-liquid equilibrium (VLE) data are provided for this binary system, and the enthalpies of vaporization of acetone and ethanol may be assumed to be constant at 29.6 and 38.9 kJ/mol, respectively. Assume that the constant-molal-overflow (CMO) assumption applies.

a. Is the CMO approximation valid?

b. Calculate the number of stages needed at total reflux. If the minimum number of stages exceeds 10, the separation is impossible.

c. Your supervisor, a distillation expert, has answered question b, and assures you that the minimum number of stages needed at total reflux is less than 10. Calculate the reflux ratio needed to achieve the desired separation. How does the reflux ratio change as the thermal state of the feed is varied?

d. If it is possible to move the feed inlet stage, would you recommend that this be done? What is the optimum feed location? How is the separation affected as the feed inlet is changed?

e. How should the design be changed if the tray efficiency decreases below unity?
2. The q-line is constructed by drawing a straight line from \((x_F, x_F)\) with a slope equal to \(q/(q - 1)\).

3. The stripping-section operating line is the straight line from \((x_B, x_B)\) to the intersection of the rectifying-section operating line and the q-line.

The function Interp is useful in implementing the operating lines and the q-lines even though all three are straight lines. For the purpose of calculating equilibrium compositions, x-y data have been entered as a table with 101 points \((x, y)\). This spacing of data points is expected to be adequate for accurate interpolation of the acetone-ethanol x-y diagram. For another system with an x-y diagram that has a more complex shape, more data points in the table may be needed.

The McCabe-Thiele diagram is constructed by “stepping off stages.” The starting point is \((x_D, x_D)\), which is the vapor composition ascending from tray 1. The liquid composition descending from tray 1 is the mole fraction in equilibrium with the vapor ascending from tray 1, which is obtained using the function Interp: 

\[ x_j = \text{Interp}(x_D, x_{\text{Data}}, y_{\text{Data}}, 0) \]

Next, the vapor composition rising from tray 2 is calculated from the rectifying-section operating line (or component-balance equation), again using Interp. The stepping off of stages continues over the entire column, switching to the stripping-section operating line at the feed tray. In this way, the entire McCabe-Thiele diagram can be computed and graphically represented using standard Excel charting capability.

Standard Excel what-if analysis capability can be used to evaluate design results. For example, Goal Seek or Solver may be used to calculate the reflux ratio to obtain the liquid composition \((x_B)\) descending from tray 10. (Solver seems to converge more reliably and accurately than Goal Seek.)

As was first suggested by Murphree, the McCabe-Thiele procedure may be made more realistic by relaxing the approximation that vapor-liquid equilibrium is achieved on each stage. The Murphrey efficiency is defined as:

\[ E_{ML} = \frac{x_j - x_{j-1}}{x_j - x_{j-1}} \] (4)

In Eq. 4, \(x_j^*\) is the liquid mole fraction that is in equilibrium with the vapor ascending from tray \(j\) and \(x_j\) is the actual mole fraction of the liquid descending from tray \(j\). As the efficiency decreases to values less than unity, the decrease in liquid mole fraction from the distillate to the bottom will be reduced. The concept of Murphree efficiency is equally applicable to the vapor or liquid phase, and here it is convenient to apply it to the liquid phase. Note that if Eq. 4 is be applied, the use of Murphree efficiencies requires a modification in the way that the liquid mole fraction is calculated from the vapor mole fraction.

It is useful to estimate heat effects consistent with the CMO approximation. Here, it is assumed that sensible heat effects and heats of mixing are negligible and that heat duties are only associated with evaporating and condensing binary mixtures based on their \((\text{fixed})\) enthalpies of vaporization. The condenser duty, \(Q_C\), is the heat removal rate required to condense a vapor with flowrate \(V\) and composition \(x_{D}\):

\[ -Q_C = V[x_D \Delta H_{vap}^1 + (1 - x_D) \Delta H_{vap}^2] \] (5)

The CMO approximation implies that the sum of the condenser and reboiler duties is zero for a saturated-liquid feed \((q = 1)\). The heat duty required to change the thermal state of the feed from the saturated-liquid state is:

\[ Q_F = F(1 - q)[x_F \Delta H_{vap}^1 + (1 - x_F) \Delta H_{vap}^2] \] (6)

The reboiler duty \((Q_R)\) is calculated from \(Q_C\) and \(Q_F\):

\[ Q_R = Q_C - Q_F \] (7)

**Evaluating binary separations**

A spreadsheet is used to analyze the separation of the acetone-ethanol mixture and other binary mixtures using the McCabe-Thiele approach.

The McCabe-Thiele diagram is constructed by interpolation of x-y data. These data may be obtained from a variety of sources, such as standard thermodynamic models or commercial process-simulation software. The advantage of this approach is that the source may be sophisticated models and databases that are difficult and time-consuming to program in Excel. However, x-y data may not always be available for the system of interest, so the use of Excel for regression of phase-equilibrium data to generate the x-y data is demonstrated here.

VLE data for the acetone-ethanol system at 50°C, 71°C and 80°C \((6, 7)\) have been used to regress the parameters of the NRTL activity-coefficient model. Since the pressure is low (about 2 bar or less), pressure effects on the liquid fugacity may be neglected and the vapor phase can be treated as an ideal gas. Thus, the total pressure of the binary mixture is given by Eq. 8, and the vapor composition for the specified liquid composition may be calculated from Eq. 9:
The Role of the McCabe-Thiele Method in Distillation Engineering

The availability of digital computers and the intense development of solution algorithms, beginning in about 1951, eliminated the need for approximate solutions in equilibrium-stage distillation calculations and enabled more rigorous simulations. A comprehensive suite of powerful rigorous methods is available today in commercial software, which has completely replaced simplified methods for the design of distillation towers. Unfortunately, these rigorous, computerized calculations are often used as a black box, and the intuitive, visualization benefits inherent in the simplified procedures are in danger of being lost. Kister noted that despite the huge progress in distillation, the number of tower malfunctions is not declining (12).

Experts recognize that an effective distillation design and analysis toolkit must have more than the capability for rigorous, computerized calculations. Accurate calculation of thermodynamic properties (especially vapor-liquid equilibriums) is crucial to producing correct designs (17). Residue curve maps (RCMs) (14) provide visualization of feasible and infeasible separation sequences, and have been extended to multicomponent systems and pressure variations. Graphical techniques, like McCabe-Thiele and Hengstebeck diagrams, multicomponent distillation profiles and RCMs, are excellent troubleshooting tools because they uncover design problems, such as composition pinches and unforgiving composition profiles (15). Good plant data are difficult to obtain, but are well worth the time and effort required to collect them, since they are the prime tool of the troubleshooter. Visualization tools capture the fundamentals of distillation. Such a diverse and comprehensive toolkit gives engineers detailed results, insight, and understanding to develop superior designs, as well as the judgment to diagnose and resolve operational problems.

Today, implementation of the McCabe-Thiele graphical procedure does not require the CMO approximation, since the diagram can easily be constructed from a rigorous distillation calculation. In addition, the McCabe-Thiele diagram has been extended to multicomponent systems by Hengstebeck. When used in this manner, McCabe-Thiele/Hengstebeck diagrams are highly effective as design and troubleshooting tools for analyzing new energy-saving technologies (16), designing steam-stripping systems (17), improving energy efficiency (18), evaluating revamp improvements (19), and explaining counter-intuitive observations in a multi-feed distillation tower (20).

“Perry’s Chemical Engineers’ Handbook” (21) states: “With the widespread availability of computers, the preferred approach to design is equation based … Nevertheless, diagrams are useful for quick approximations, for interpreting results of equation-based methods, and for demonstrating the effect of various design variables. The x-y diagram is the most convenient for these purposes.”

\[ P = P_{1}^{\text{sat}} x_1 \gamma_1 + P_{2}^{\text{sat}} x_2 \gamma_2 \]  
\[ \gamma_1 = \frac{P}{P_{1}^{\text{sat}}} x_1 \gamma_1 \]

Any suitable activity-coefficient model may be used to represent the liquid nonideality, and here the NRTL model has been chosen:

\[ \frac{G^E}{x_1 x_2 R T} = \frac{G_{21} \tau_{21}}{x_1 + x_2 G_{21}} + \frac{G_{12} \tau_{12}}{x_2 + x_1 G_{12}} \]

\[ G_{12} \equiv \exp(-\alpha \tau_{12}) \quad \text{and} \quad G_{21} \equiv \exp(-\alpha \tau_{21}) \]

\[ \tau_{12} = A_{12} + B_{12} / T \quad \text{and} \quad \tau_{21} = A_{21} + B_{21} / T \]

The equations for the resulting activity coefficients (\( \gamma_1 \) and \( \gamma_2 \)) are available in standard references. At each temperature, the vapor pressures of acetone and ethanol have been estimated using the function Interp and assuming that the logarithm of the vapor pressure is linear in reciprocal temperature.

The optimum values of the NRTL parameters \((A_{12}, A_{21}, B_{12} \text{ and } B_{21})\) have been determined using Solver to minimize the sum-squared error between the measured and calculated total pressures \((i.e., \text{ Barker’s method})\).

The optimum values of the NRTL parameters are:

\[ \alpha = 0.3; A_{12} = 0.724358; B_{12} = -159.176; A_{21} = -2.33876; B_{21} = 921.128. \]

Using the NRTL model with Eqs. 8–12, an x-y diagram is generated. At each value of \( x \), the temperature must be found such that the total pressure (Eq. 8) is equal to the stage pressure (constant at 1 atm or 101.325 kPa). Although Goal Seek may be used to solve this equation, it is tedious, since the calculation will have to be repeated 101 times. A better approach is to calculate the sum-squared error of the difference between the calculated pressures and 101.325 kPa, and then use Solver to minimize the sum-squared error by changing the 101 cells that contain the temperatures corresponding to the liquid compositions. The latter methodology (provided with the online article) is efficient in terms of human effort, since a single Excel step generates the entire x-y table.

Total reflux

The total-reflux calculation, which corresponds to infinite reflux ratio, is useful because it determines the minimum number of stages needed for the target separa-
Reactions and Separations

Figure 2. Acetone-ethanol separation at 1 atm and total reflux requires between six and seven stages to achieve $x_D = 0.09$ and $x_B = 0.03$.

At infinite reflux, both operating lines reduce to the diagonal ($x = y$) line. The total-reflux diagram for acetone-ethanol is presented as Figure 2, which indicates that between six and seven stages are needed to achieve $x_D = 0.9$ and $x_B = 0.03$. Hence, it is possible to use a distillation column with 10 stages for the desired separation.

Effect of $q$ and comparison with rigorous calculation

Figure 3 presents the reflux ratio needed to achieve the desired separation. As shown in the figure, the desired reflux ratio is readily calculated using Solver to determine the reflux ratio that gives the target bottom concentration, $x_B = 0.03$.

Figure 3 demonstrates that the optimum feed location is tray 6 rather than tray 5, but the penalty for the non-optimum feed location is fairly small.

A study of the effect of varying the thermal state of the feed is summarized in Table 1 (using the optimum feed location, tray 6). The required reflux ratio decreases as the thermal state of the feed ($q$) increases, and the reboiler duty ($Q_R$) increases as $q$ increases. The reboiler duty in Table 1 is not the entire heat load, since it does not include any heat treatment of the feed. Thus, the table includes $Q_R + Q_F$, where $Q_F$ is the heat load required to modify the thermal state of the feed from $q = 1$ (saturated liquid). (Based on the Lewis CMO approximation, $Q_R + Q_F$ is exactly equal to $-Q_C$.) On this basis, the total heat load decreases as $q$ increases.

The analysis demonstrates that the effect of an increase in $q$ results in a decrease in capital costs (due to a lower reflux ratio and column flows and hence a smaller column diameter), as well as a decrease in operating costs (mainly a lower heating duty, which is usually the major operating cost). The value of this analysis is that the design engineer can easily understand the benefits of varying $q$ and make the best design choice.

This McCabe-Thiele method was tested by comparing its calculated $q$ variations with rigorous results from the Aspen Plus process simulator. The Aspen Plus simulation uses the same thermodynamic model (ideal vapor phase, no pressure effects on the liquid fugacity, and the NRTL activity-coefficient model), but rigorously deals with heat effects. It does not make the Lewis approximations (constant molal overflow or constant heat of vaporization even as the liquid composition changes, and negligible sensible
heat and heat of mixing), and hence provides a way to estimate the errors caused by the approximations.

Figures 4 and 5 indicate that the Lewis approximations cause errors of about 10% in the reflux ratio and up to 15% in the reboiler duty. The Lewis approximations are in excellent agreement with the rigorous calculation for the liquid composition profile (Figure 6), but poor agreement with the rigorous calculation for the flow profiles (Figure 7).

Today, rigorous calculations rather than shortcut methods are used for detailed design of distillation columns. However, Figures 4 and 5 clearly demonstrate that the McCabe-Thiele method captures the trends reasonably well, and hence remains important for understanding the foundations of distillation engineering. As discussed in the sidebar on p. 39 (“The Role of the McCabe-Thiele Method in Distillation Engineering”), the McCabe-Thiele diagram, without the CMO approximation, has excellent present-day value as a design and troubleshooting tool.

**Effect of feed location**

Figure 8 shows the effect of nonoptimum feed tray location on the required reboiler duty. Note that a severely nonoptimum feed location (e.g., tray 9 vs. tray 6) will require the reboiler duty to be doubled in order to achieve the target separation. Figure 9 illustrates the pinch point that occurs when the feed point is too low. Figure 10 provides further illustration of the pinch point, showing that the liquid mole fraction reaches an asymp-
Reactions and Separations

totic value of about 0.09 at tray 9, and the addition of more stages above the feed will have no effect on improving product purities.

The Excel file can be used to further study the analogous detrimental effect that occurs if the feed point is too high.

Effect of reduced tray efficiency

It is usually recommended that the sectional column efficiency be defined as the ratio of the theoretical number of stages to the actual number of stages to achieve a particular separation (8). Since efficiencies vary from one section to another, it is best to apply the efficiency separately for each section (i.e., rectifying and stripping).

The concept of Murphree efficiency ($E_{ML}$, Eq. 4) has been used to investigate the effect of tray efficiency. Table 2 and Figure 11 show that the required reflux ratio and the resulting reboiler duty increase substantially as $E_{ML}$ decreases below unity. Note also that the optimum feed location changes as efficiency changes, although the results are insensitive to the feed location when the reflux ratio is high.

Figure 12 presents the McCabe-Thiele diagram for the case where $E_{ML} = 0.7$. The reduced Murphree efficiency effectively reduces the relative volatility, which makes the separation more difficult, requiring a higher reflux ratio. In fact, the desired separation is barely possible for $E_{ML} = 0.67$, and further reduction in the efficiency will make the desired separation impossible, even at total reflux.

It should be emphasized that the Murphree efficiency is only a crude description of the performance of real trays, and hence the effect of varying $E_{ML}$ should be interpreted with caution. The effects shown here are only qualitatively applicable, but useful to illustrate the effects of reduced tray efficiency.

Solution to the acetone-ethanol example problem

a. Constant molal overflow is a reasonably good approximation even for this case, where the enthalpy of vaporization of ethanol is 32% higher than that of acetone. The CMO approximation is especially useful because it captures trends, and thus serves as an aid to understand the fundamentals of distillation engineering. But CMO does not yield reliably accurate results, and is not recommended for detailed design calculations, especially since software employing rigorous methods is widely available.

b. The number of stages needed at total reflux is between six and seven. Thus, the available 10-stage column is likely to be adequate for the desired separation.

c. The reflux ratio needed for the specified separation is 2.0. The reflux ratio decreases with increasing $q$, and the required heat duty decreases as $q$ increases. Therefore, it is preferable to operate the column at high values of $q$.

d. The existing feed location (tray 5) is only slightly suboptimal, with a required reflux ratio of 2.0, compared with 1.9 if the feed location is lowered to tray 6. Figure 8 shows the negative effects that will occur for a poorly located feed stage.

e. The separation becomes far more difficult as $E_{ML}$.
decreases below unity (Figure 11). Note also that low values of $E_{ML}$ may cause pinch points that do not exist at higher efficiencies.

Other binary separations

Other binary systems may easily be studied by replacing the $x$-$y$ table used here for the acetone-ethanol binary mixture. The Excel file supplied online provides two additional examples of $x$-$y$ diagrams for binary systems.

The first example is representative of the benzene-toluene system and assumes constant relative volatility, $\alpha$:

$$
\alpha \equiv \frac{y/x}{(1-y)/(1-x)} \quad (13)
$$

$$
y = \frac{xa}{1 + (\alpha - 1)x} \quad (14)
$$

The value of the simple constant-$\alpha$ system is that the effects of close-boiling and wide-boiling systems may easily be studied. Detailed study of this system is left as an exercise for the reader.

In the second example, $x$-$y$ data from an external source are used — $x$-$y$ data for the ethanol-water binary system at 1 atm from the Aspen Plus process simulator. The McCabe-Thiele diagram indicates that (1) a reflux ratio of 5.4 is required for the target separation, and (2) the optimum feed tray is low in the column because the separation is very difficult at high ethanol concentrations due to the formation of an azeotrope (at $x \approx 0.9$). Hence, more stages are needed above the feed stage. The reader is urged to perform another calculation by increasing $x_D$ slightly, from 0.83 to 0.84 (leaving $x_F$ unchanged at 0.01). The required reflux ratio almost doubles (to 10.2), which decreases below unity (Figure 11). Note also that low values of $E_{ML}$ may cause pinch points that do not exist at higher efficiencies.

<table>
<thead>
<tr>
<th>Nomenclature</th>
</tr>
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<tbody>
<tr>
<td>$A_{12}, A_{21}, B_{12}, B_{21}$ = temperature-dependence parameters in NRTL model (Eq. 12)</td>
</tr>
<tr>
<td>$B$ = bottom flowrate, kmol/h</td>
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<tr>
<td>$D$ = distillate flowrate, kmol/h</td>
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<tr>
<td>$E_{ML}$ = Murphree efficiency, applied to the liquid compositions (Eq. 4)</td>
</tr>
<tr>
<td>$G^E$ = excess Gibbs energy (Eq. 10)</td>
</tr>
<tr>
<td>$G_{12}, G_{21}$ = terms in NRTL model (Eqs. 10 and 11)</td>
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<tr>
<td>$\Delta H_{1}^{vap}, \Delta H_{2}^{vap}$ = enthalpy of vaporization of components 1 and 2, kJ/mol</td>
</tr>
<tr>
<td>$L$ = liquid flowrate in rectifying section, kmol/h</td>
</tr>
<tr>
<td>$\bar{L}$ = liquid flowrate in stripping section, kmol/h</td>
</tr>
<tr>
<td>$P$ = pressure, kPa</td>
</tr>
<tr>
<td>$p_{1,sat}, p_{2,sat}$ = vapor pressures of components 1 and 2, kPa</td>
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<tr>
<td>$q$ = liquid fraction or thermal state of the feed; $q = 1$ corresponds to saturated liquid</td>
</tr>
<tr>
<td>$Q$ = heat rate, GJ/h</td>
</tr>
<tr>
<td>$R$ = gas constant</td>
</tr>
<tr>
<td>$R$ = reflux ratio</td>
</tr>
<tr>
<td>$T$ = temperature, K</td>
</tr>
<tr>
<td>$V$ = vapor flowrate in rectifying section, kmol/h</td>
</tr>
<tr>
<td>$\bar{V}$ = vapor flowrate in stripping section, kmol/h</td>
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<tr>
<td>$x$ = liquid mole fraction (of the more-volatile component)</td>
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<tr>
<td>$x^*$ = liquid mole fraction in equilibrium with $y$ (Eq. 4)</td>
</tr>
<tr>
<td>$y$ = vapor mole fraction (of the more-volatile component)</td>
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</tbody>
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<table>
<thead>
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<th>Greek Letters</th>
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<tbody>
<tr>
<td>$\alpha$ = nonrandomness parameter in NRTL model (Eq. 11)</td>
</tr>
<tr>
<td>$\alpha$ = relative volatility (Eq. 13)</td>
</tr>
<tr>
<td>$\gamma_1, \gamma_2$ = activity coefficients of components 1 and 2</td>
</tr>
<tr>
<td>$\tau$ = interaction-energy parameter in NRTL model (Eq. 10)</td>
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<table>
<thead>
<tr>
<th>Subscripts</th>
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<tbody>
<tr>
<td>1, 2 = components 1 and 2</td>
</tr>
<tr>
<td>$B$ = bottom</td>
</tr>
<tr>
<td>$C$ = condenser</td>
</tr>
<tr>
<td>$D$ = distillate</td>
</tr>
<tr>
<td>$F$ = feed</td>
</tr>
<tr>
<td>$j$ = stage number</td>
</tr>
<tr>
<td>$R$ = reboiler</td>
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Reactions and Separations

highlights the difficulty of achieving higher product purity in the vicinity of the azeotrope. The visual approach clearly provides insight and understanding of the special considerations required for the purification of a mixture that forms an azeotrope.

Closing thoughts

The ability to easily vary input specifications in the Excel spreadsheet and to visualize the effects on column performance has significant value in teaching distillation fundamentals. Engineers are better able to grasp the effects of various inputs, and they become better design engineers and more competent, discriminating users of commercial software. The understanding gained from the spreadsheet is a valuable first step in using a rigorous simulation as a design and troubleshooting tool.

But how robust is the McCabe-Thiele approach, which is the foundation of this Excel application? In particular, can it give results that will confuse or even mislead? In the author’s experience, the McCabe-Thiele approach captures trends well and thus is a valid and useful teaching tool.

So, should this tool be extended to improve accuracy by eliminating the poor approximations and thus become applicable to more realistic distillation situations (e.g., heat effects, complex column configurations, multi-component systems, mass transfer limitations, chemical reactions and kinetics, etc.)? Extensions should be limited and should be done with caution. Rigorous modeling methods are very powerful for describing real distillation systems. The computer code based on these methods supports flexible design requirements very well. Thus, the best use of the spreadsheet method presented here is to produce engineers who understand the fundamentals, have good engineering judgment, and become discriminating users of sophisticated detailed methodologies.

As Kister noted, “the two can coexist” (4). In fact, it is good practice to benefit from both the accuracy and flexibility of rigorous calculations and the insight and understanding gained by visualization of the venerable McCabe-Thiele diagram.

Literature Cited


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