Distillation Design
The McCabe–Thiele Method
Distiller diagram
Introduction

• Using rigorous tray–by–tray calculations is time consuming, and is often unnecessary.
• One quick method of estimation for number of plates and feed stage can be obtained from the graphical McCabe–Thiele Method.
• This eliminates the need for tedious calculations, and is also the first step to understanding the Fenske–Underwood–Gilliland method for multi–component distillation
• Typically, the inlet flow to the distillation column is known, as well as mole percentages to feed plate, because these would be specified by plant conditions.

• The desired composition of the bottoms and distillate products will be specified, and the engineer will need to design a distillation column to produce these results.

• With the McCabe–Thiele Method, the total number of necessary plates, as well as the feed plate location can be estimated, and some information can also be determined about the enthalpic condition of the feed and reflux ratio.
• This method assumes that the column is operated under constant pressure, and the constant molal overflow assumption is necessary, which states that the flow rates of liquid and vapor do not change throughout the column.

• To understand this method, it is necessary to first elaborate on the subjects of the x–y diagram, and the operating lines used to create the McCabe–Thiele diagram.
The x–y diagram

• The x–y diagram depicts vapor–liquid equilibrium data, where any point on the curve shows the variations of the amount of liquid that is in equilibrium with vapor at different temperatures.

• In a binary system containing substances A and B, a point on the equilibrium curve can be separated into the mole percentage of the vapor that is substance A on the y axis and the mole percentage of the liquid that is substance A on the x axis.
Relative volatility

- The relative volatility can be considered constant and the following equation can be used.
  \[ \alpha_{ij} = \frac{y_i}{x_i} \]

- When considering a binary system, the previous equation can be simplified.
  \[ \alpha_{ij} = \frac{y_i}{x_i} \cdot \frac{1}{(1-x_i)} \]
• Knowing the relative volatility for a system is also useful in determining the amount of separation possible.

• A relative volatility of 1 indicates that both components are equally volatile and no separation takes place, and when the relative volatility is low, (a < 1.05), separation becomes difficult and expansive because a large number of trays are required.

• The higher the relative volatility, or the lower the pressure, the more separable are the two components; this connotes fewer stages in a distillation column in order to effect the same separation between the overhead and bottoms products.
x–y diagram and operating lines

• Create the x–y diagram of the two-component system and add the x=y (diagonal) line.

• Specify the purity of the top and bottoms products, as well as the feed plate condition (xD,xB,and zF, respectively).

• Draw the operating lines by meeting one of the following
Operating line in rectifying section

- Portion of the distillation column above the feed is called the rectifying section.
- If it is assumed that the heat of mixing is negligible and that the difference in the molar latent heats of vaporization of the binary system also differs by a negligible amount, then the observed relationship between any two passing streams is simplified to:

\[ y = \frac{L}{V} x + \frac{x_D D}{V} \]
\[ y = \text{mole fraction of more volatile component in the vapor} \]
\[ x = \text{mole fraction of more volatile component in the liquid} \]
\[ x_D = \text{mole fraction of more volatile component in the distillate} \]
\[ D = \text{Distillate product flow (mol/t)} \]
\[ L = \text{total flow rate of the liquid stream in the rectifying section (mol/t)} \]
\[ V = \text{total flow rate of the vapor stream in the rectifying section (mol/t)} \]

This is known as the operating line for the rectifying section, or the upper operating line, in short. Remembering that the x–y diagram is a plot of vapor (V) vs. liquid (L), it can be seen that the operating line is a simple \( y = mx + b \) equation. Therefore, with the point \((x_D, y_1)\) and the slope \((L/V)\), this operating line can be plotted.
Operating line in stripping section

- Portion of the distillation column below the feed is called the stripping section. With the previously stated assumptions,
- The observed relationship between any two passing streams is simplified to:

\[ y = \frac{L}{V} x - \frac{x_B B}{V} \]
y = mole fraction of more volatile component in the vapor
x = mole fraction of more volatile component in the liquid
xB = mole fraction of more volatile component in the bottom product
B = Bottom product flow (mol/t)
L = total flow rate of the liquid stream in the rectifying section (mol/t)
V = total flow rate of the vapor stream in the rectifying section (mol/t)

This is known as the operating line for the stripping section, or the lower operating line, in short. Again, it can be seen that this is a simple line equation with the slope \((L/ V)\). With the slope and point where \(x_D\) meets the diagonal, the lower operating line can be plotted.
Feed–Line Equation

- A third useful equation is the Feed–Line Equation, commonly known as the q–line.
  - \( q = \) mole fraction of saturated liquid in feed stream
  - \( x = \) mole fraction of any component in the liquid
  - \( z_F = \) mole fraction of any component in the feed

- It represents the intersection of the upper and lower operating lines. The stage that crosses the q–line is the optimum feed plate.
Position A:
q > 1.0
subcooled liquid

Position B:
q = 1.0
saturated liquid

Position C:
0 < q < 1
mixture of saturated vapor and liquid

Position D:
q = 0
saturated vapor

Position E:
q < 0
superheated vapor
• Two possible feed conditions, saturated liquid and saturated vapor.
• Notice how the slopes of the upper and lower operating lines do not change, but the number of necessary stages changes due to feed conditions
• Saturated Vapor: Slope of the q–line is zero, Direction of the q–line is horizontal
• Saturated Liquid: Slope of the q–line is infinity, Direction of the q–line is vertical
• If the slope of the $q$–line is not directly known, it may be helpful to look at the feed plate enthalpic conditions.

• $HV = \text{enthalpy per mol of vapor}$
  $hl = \text{enthalpy per mol of liquid}$
  $hF = \text{enthalpy per mol of feed}$
Slope of the q-line and the rectifying section

- Draw the two known operating lines from the known slopes.
- The stripping section line can be drawn between the points where the known operating lines intersect and the point where XB meets the diagonal line.
- On the graph to the right, the rectifying section operating line is red (upper section), the q-line is blue and the stripping section is green (lower section)
Information about the reflux ratio

- The use a limiting condition, there will be two possibilities: only the slope of the q-line will be necessary, or no further information will be necessary.

- The McCabe–Thiele method allows full control over reboiler duty, and it is not uncommon to first solve a problem assuming minimum reflux ratio. Results can be scaled to actual reflux ratio, typically $R = 1.4 \times R_{\text{min}}$. 
Maximum Reflux

- The condition of total reflux implies that both the upper and lower operating lines are situated on the diagonal.
- This is as far as the operating lines can be removed from the equilibrium curve, and therefore, the maximum separation possible is occurring at each stage.
- Further, this correlates to the minimum number of equilibrium stages necessary to reach the desired purity. The column is at maximum diameter, but there is no product because all of the overhead product is being returned to the column as reflux.
Minimum Reflux

• This is a conceptual limit, as it implies that the entering and exiting streams of the stage are in equilibrium, and it would take an infinite number of stages to accomplish this.

• When a McCabe–Thiele diagram is graphed using the condition of minimum reflux, the slope of the upper operating line is no longer necessary.

• Instead, the upper operating is drawn as the line between the point \((x_D, y_1)\) and where the q–line meets the equilibrium curve. At this condition, infinite stages are necessary.
Draw the stages

- Shown in purple, starting at xD on the diagonal line, move horizontal to the equilibrium line, and then vertically back to x–y line (see graph).
- Continue process toward xB, switching the lower operating line after crossing the q–line, estimating the last stage if necessary.
- The optimum feed plate is one which crosses the q–line. In the example, there are four stages, and the optimum feed plate is number three.
- This procedure finds the theoretical number of plates, if all equipment was 100% efficient. In reality, an efficiency factor should be specified to represent a real system.
- One efficiency factor is the overall efficiency, where the theoretical plates are a percentage of the real plates:
Summary of Steps

- Draw x–y diagram and x=y line
- Find the outlet and feed conditions known
- Draw q–line
- Draw upper operating line
- Connect lower operating line
- Step stages from known end conditions, and count stages