At undergraduate level, the separation of binary mixtures is studied using, mainly, the McCabe-Thiele Method because of the advantage to present the results in graphical form. However, most of the applications are limited to problems where extreme (top and bottom) compositions and reflux ratio are specified and the objective is to determinate the number of stages. By the use of McCabe-Thiele Method and the advantage of a solve-package (Mathcad™) a procedure is proposed to solving problems with different specifications. Unlike the traditional application, the number of stages can or can not be specified. Depending on the available information, the objective can be the one of determining top or bottom composition and reflux ratio, for instance. The proposed procedure allows a detailed analysis of the separation, avoiding the cycle “right solution or wrong solution”. The proposed procedure is also valid for columns with multiple feeds and can be implemented by using other softwares.

**Keywords** – Distillation – McCabe-Thiele Method – Undergraduate – Mathcad™

1. Introduction

Distillation is one of the most important separation processes used in chemical and petrochemical industries due to its great efficiency in separating different types of mixtures. Therefore, chemical engineering curriculum covers one or more courses involving this subject, which always consider binary mixtures to begin with.

As computer codes have become more popular solution of problems involving distillation calculations has been brought to pass by using more powerful and efficient softwares (Aspen™, Hysys™, Design™, etc.). However, graphic methods for dealing with problems like those provide a preliminary overview followed by a deeper understanding of the distillation process, which are fundamental pre-requisites to initiate the studies on the separation of multi component mixtures. Besides, the softwares mentioned above are a very expensive part of any budget such that not everyone can have access to those tools.

Among all graphic methods the most popular are McCabe-Thiele and Ponchon-Savarit Methods (Henley and Seader, 1981; King, 1971; Kister, 1990). These methods differ one another because the later considers the energy balance by using enthalpy diagrams. At undergraduate level is common to consider ideal phases, both liquid and vapor, in the process, which makes the supposition of constant molar flow throughout the section true and turns the McCabe-Thiele Method into one of the most widespread used methods.

In most of the applications involving the McCabe-Thiele Method if the characteristics of the feed (composition and thermal condition) to the distillation column are given, top and bottom composition are
specified as well as the reflux ratio. Another very common application of this method occurs when the recovery ratio of one of the components, the specification of bottom or top composition, and the reflux ratio are given. That is, traditionally the McCabe-Thiele Method is used just to determine the number of stages to achieve a specified separation.

The fact that the McCabe-Thiele Method has been used mainly to determine the number of stages is due to, in a recent past, problems involving this subject were solved by hand (means of grid paper). For a given problem, the equilibrium curve along with the operation lines was plotted and then the number of stages was obtained. All of those tasks were done manually. For every new operational condition like for example a modification in the reflux ratio, all the steps had to be repeated.

By using the commercial software Mathcad™ a procedure to solve distillation problems with different specification cases is presented. According to this procedure the number of stages can be fixed and depending on the available inputs to the system the objective can be, for example, to determine the top or bottom composition or moreover to calculate the reflux ratio.

The procedure can be extended to other applications involving distillation columns with multiple feed points. In the examples presented in this paper the necessary information about composition and thermal condition of the feed are available. The total condensation of the top is also assumed.

2. Determining the Number of Stages

In this typical case, the information about top and bottom composition and the reflux are available. The objective is to determine the number of stages. In order to perform this task the procedure looks for the feed line (Eq. 1), rectification line (Eq. 2), and stripping line (Eq. 3) in a y-x diagram and then it computes the number of stages.

\[
y = \frac{q}{q-1} x - \frac{z}{q-1}
\]

\[
y = \frac{R}{R+1} x + \frac{x_D}{R+1}
\]

\[
y = \frac{\bar{L}}{\bar{V}} x - \frac{B x_B}{\bar{V}}
\]

In Figure 1 a McCabe-Thiele drawing that ended up in an eight-stage column with the feed at the fourth stage (the stages are numbered from bottom to top) can be seen. It is also observed that the number of stages is more than enough to achieve the specification since the last stage presents a composition higher than \(x_D\). Therefore, the top product composition is different from that which has been specified. In fact, if the reflux ratio was manipulated, the desired separation could be obtained by using seven stages.

![Fig. 1 Typical application of the McCabe-Thiele Method: calculating the number of stages. \(z=0.5, q=0.5, x_D=0.95, x_B=0.05, \alpha=3, \) and \(R=2.5\).](image)

3. Determining the Reflux Ratio

The first application of the proposed procedure is to be used in problems in which top or bottom composition and the number of
stages are specified, and the objective is to determine the reflux ratio.

In Figure 2 the Mathcad™ code used to deal with problems with this kind of specification is shown. Objectively speaking, this code can be described as following:

- Giving inputs to the problem;
- Determining the top and bottom flow rates;
- Defining the operation lines (rectification and stripping sections), feed point, diagonal line, and equilibrium curve;
- Defining a objective function (McCabe-Thiele Method), which is minimized by the internal Mathcad™ Minimize function (Conjugate Gradient Method);
- Defining the constraints on the intersection between the stripping line, stripping line, and rectification line;
- Defining the constraints on the intersection between the stripping line and the diagonal;
- Defining the constraints on the intersection between the rectification line and the diagonal;
- Defining the constraints on the ratio between the rectification flow rate and the stripping flow rate;
- Minimizing the objective function;
- Drawing the McCabe-Thiele plot.

If the previous code is to be compared to a traditional application then it can be said that it presents as a differential the fact that the rectification and stripping lines are drawing as a function of the unknown variables reflux ratio, liquid and vapor flow rate in the rectification section, and bottom composition. That is exactly the idea of defining an objective function.

The reason for an objective function is to compare the top composition obtained from determining the unknown variables with the specified value given as an input to the problem. In short, the procedure can be read as: once the constraints are fulfilled, find the values of the unknown variables such that the objective function is minimized. Needless to say, the minimization problem is bound by the determination of four variables, which turns the computation sensible to initial guesses. This means that the final value of the objective function has to be always taking into account.

Inputs
\[ F = 100 \quad x_D = 0.5 \quad q = 0.5 \quad N = 7 \quad x_I = 0.2 \quad x_B = 0.65 \quad x_L = 0.45 \]

Computing top and bottom flow rates
\[
\begin{align*}
D & = 30 \\
B & = 30 \\
V_D & = D \cdot x_D + B \cdot x_B \\
V_B & = D \cdot x_B + B \cdot x_B
\end{align*}
\]

Defining operational, equilibrium, and diagonal lines
\[
\begin{align*}
\text{McCabe (Ref. Lb, Vb, x_n)} & : \quad \text{yfeed(x) = } \frac{q \cdot x - x_D - x_D}{\text{Refl} - 1} \\
\text{Vb} & = \text{Vb} \text{ (Ref. Lb, Vb)} \\
\text{Lb} & = V_B - B \cdot \text{Refl} \\
\text{Refl} & = 100
\end{align*}
\]

Defining the objective function
\[
\begin{align*}
\text{McCabe (Ref. Lb, Vb, x_n)} & : \quad \text{yfeed(x) = } \frac{q \cdot x - x_D - x_D}{\text{Refl} - 1} \\
\text{Vb} & = \text{Vb} \text{ (Ref. Lb, Vb)} \\
\text{Lb} & = V_B - B \cdot \text{Refl} \\
\text{Refl} & = 100
\end{align*}
\]

Method
\[
\begin{align*}
\text{McCabe (Ref. Lb, Vb, x_n)} & : \quad \text{yfeed(x) = } \frac{q \cdot x - x_D - x_D}{\text{Refl} - 1} \\
\text{Vb} & = \text{Vb} \text{ (Ref. Lb, Vb)} \\
\text{Lb} & = V_B - B \cdot \text{Refl} \\
\text{Refl} & = 100
\end{align*}
\]

Fig. 2 Mathcad™ code used to determine the reflux ratio.
It can be seen in Figure 3a the situation in which the minimization problem does not fulfill the constraint of matching the number of stages between the top and bottom compositions. Figure 3b presents the McCabe-Thiele Method where the top and bottom compositions match properly the specified number of stages. The reflux ratio necessary to achieve the right configuration is about 3.1458, using the fourth stage as the feed stage.

The procedure can be implemented by writing the code in languages like Fortran, Matlab® or even the Mathcad™ itself. For didactic reasons the authors choose to use the internal routines of Mathcad™.

4. Determining the Bottom Composition

In this application, information about the distillate composition and reflux ratio is available as well as the number of stages. In Figure 4 is presented the Mathcad™ code used to solve the problem of finding the top composition.

![Fig. 3 Non-typical application of McCabe-Thiele Method: calculating the of reflux ratio. z=0.5, q=0.5, xD=0.95, xB=0.05, α=3, and N=7.](image)

![Fig. 4 Mathcad™ code used to determine the bottom composition.](image)
The procedure to be followed is quite similar to that one presented in the previous chapter. The difference in this case is that the top and bottom flow rates can not be determined. On the other hand, the intersection between the feed and rectification lines can be calculated.

By comparing the codes in Figures 2 and 4 it can be observed that in both cases there exist four variables to be determined. The main difference lies on the definition of the operation lines. In Figure 3 the rectification line has the reflux ratio as the variable to be found while in Figure 4 all the variables are part of the stripping line.

In terms of convergence the case shown in Figure 4 is more stable than that of Figure 2. In other words, when the information about rectification and stripping lines are not available the number of solutions appears to be larger and not all solutions computed by the minimization subroutine are physically attainable.

Problems involving other specification inputs can be handled by using similar codes like those presented in Figure 2 and 4. For example, determining the top composition having the reflux ratio and bottom composition as inputs. In any case in order to minimize the objective function there always be four variables to be determined regardless of the specification inputs.

5. Conclusions

A procedure used to extend the applications of McCabe-Thiele Method to distillation problems was presented. Furthermore, the basic idea was to express its competitiveness and broadness.

By analyzing the cases presented one can conclude that this procedure can be used in more complex applications, instead of simply determining numbers of stages in distillation columns. At the end one has managed to achieve a critical analysis of a given problem and this is a significant part in the formation of any chemical engineer.

The proposed procedure can be implemented by using other softwares such as Matlab™, Mathematica™, and Maple™. This means there are several opportunities to make use of computational resources in applications like that and any effort to take advantage of this should be always attempted. However, it is very important that the softwares quoted above be made more and more public at the undergraduate level.

Symbols

- \( B \) – Bottom flow rate
- \( L \) – Liquid flow rate below the feed stage
- \( N \) – Number of stages
- \( q \) – Parameter used to define the thermal condition of the feed.
- \( R \) – Reflux ratio
- \( V \) – Vapor flow rate below the feed stage
- \( x \) – Liquid phase mole fraction
- \( x_D \) – Top product mole fraction
- \( x_B \) – Bottom product mole fraction
- \( y \) – Vapor phase mole fraction
- \( z \) – Feed mole fraction
- \( \alpha \) – Relative volatility

References

Henley, E. J. and Seader, J. D., Equilibrium-Stage Separations Operations in Chemical Engineering, John Wiley & Sons, 1981.
