Binary Distillation Column Design Using Mathematica

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Abstract. The accurate design of distillation columns is a very important topic in chemical industry. In this paper, we describe a Mathematica program for the design of distillation columns for binary mixtures. For simplicity, it is assumed that the columns are designed by following McCabe-Thiele's procedure, a graphical method which determines both the number of stages required for the desired degree of separation and the location of the feed tray. Then, some other relevant column parameters (such as the height and diameter of the column, for example) are also determined. All results are obtained from an adequate combination of symbolic and numerical calculations taking advantage of the symbolic, numerical and graphical Mathematica programming tools. We remark that the same approach can be applied to any other kind of distillation columns by simply replacing our assumptions by those of each specific case. The performance of this program is shown through some illustrative examples. Finally, potential applications to both teaching and industry are also discussed.

1 Introduction

Nowadays it is unanimously recognized that chemical industry plays a basic role in our current technological and industrial development. Very recently, it has been reported that chemical industry represents a 455-billion-dollar-a-year business and their markets are rapidly expanding worldwide everyday. Its spectrum of products includes cosmetics and beauty products, pharmaceuticals, health care products, food additives, liquors and many others. Perhaps, the most typical example that comes to our minds is the gasoline we pump for our cars almost daily. This gasoline is obtained from crude oil by distillation, undoubtedly one of the most important processes in chemical industry [2].

From the manufacturing point of view, distillation is the most common separation technique. For example, it is the basic ingredient in the oil refining process to make gasoline, kerosene, diesel fuel, heating oil, chemicals of various grades for making plastics and other polymers, etc. This process is performed through distillation columns, which are designed to achieve this separation efficiently. However, they consume enormous amounts of energy, often contributing to more

than 50% of plant operating costs [9]. From this, it becomes clear that the correct design of distillation columns is a very important question in industry.

Traditionally, the design of distillation columns has been a numerical task: during the last three decades many numerical programs have been developed on a number of standard programming languages such as Pascal, C++ or Visual Basic, general-purpose numerical packages, such as Matlab [5] or Web-oriented tools such as Java applets [3]. They are generally based on the idea of manipulating a relatively large number of look-up table numerical data obtained from experiments and then interpolating them to obtain the vapor-liquid equilibrium (VLE) curve, which is actually the starting point of the different distillation column design methods. As a second step, an approximation of the different equilibrium rate equations is calculated. However, it has been reported that the determination of some column parameters (such as the number of trays or their location, to quote only two examples) can be very susceptible to a great variety of errors, yielding a more expensive column due to an incorrect design.

Perhaps the most natural solution to overcome this problem is to consider a symbolic approach. In fact, in the last few years computer algebra systems (CAS) become one of the most exciting tools for scientific computing. One of the most remarkable features of these computer algebra systems is their ability to integrate very powerful numerical, symbolic and graphical capabilities within a uniform framework. This feature is specially interesting because the current CAS are not able to give analytical solutions for all the equilibrium rate equations and hence, an adequate combination of numerical and symbolic procedures must be considered instead.

In this paper, we describe a Mathematica program for distillation column design. Of course, there are many types of distillation columns, each designed to perform specific types of separations, and each design differs in terms of complexity. For simplicity, in this paper we restrict ourselves to the case of continuous distillation columns for binary mixtures. It should be remarked, however, that our approach is very general in the sense that it can be applied to any other kind of distillation columns by simply replacing our assumptions by those of each specific case. In our example, we assume that the columns are designed through McCabe-Thiele's procedure. This is a graphical method which determines the number of stages required for the desired degree of separation and the location of the feed tray as functions of some parameters of the problem. The program is general enough to analyze a number of different mixtures under different conditions as well as the role of many relevant parameters of this process. To this end, an adequate combination of symbolic and numerical calculations is achieved. From these calculations, both numerical and graphical outputs are obtained. As shown later, the graphical output is actually a Mathematica movie of McCabe-Thiele's diagram. Finally, the performance of the design method is shown through some illustrative examples.

The structure of the paper is as follows: in Section 2 we introduce some basic concepts and the terminology to be used throughout the paper. Then, Section 3 gives a brief summary of McCabe-Thiele's method. In Section 4 an illustrative

example is described in detail. In addition, some comments on the implementation process are also given. Finally, the paper closes with the conclusions and some further remarks.

2 Distillation: Basic Concepts and Terminology

According to [2], *distillation* is simply defined as a process in which a liquid or vapor mixture of two or more substances is separated into its component fractions of desired purity, by the application and removal of heat. The main purpose of distillation is to separate a mixture of several components (water and alcohol, for instance) by taking advantage of their different volatilities. For example, the water boils at 100°C while alcohol boils at only 78.5°C . In this case, distillation consists of heating this water-alcohol mixture until its more volatile component (alcohol) passes into the vapor phase. As a consequence, the vapor that rises is richer in alcohol and poorer in water than the liquid from which it came. After this heating stage, this vapor is cooled to recover such component in liquid form by condensation.

If the difference in volatility (and hence in boiling point) among the components is great, complete separation may be easily accomplished by a single distillation; otherwise, several redistillations could be required. For example, the vapor from a single-stage water-alcohol distillation is not actually pure alcohol: to obtain a 50 % solution (common for whiskey), the distillate must be redistilled once or twice, and if industrial (95 %) alcohol is desired, many redistillations are needed.

Distillation is performed through many different types of distillation columns. Two examples of distillation columns are shown in Figure 1. Basically, they can be classified into *batch columns* (the feed to the column is introduced batch-wise) and the most common *continuous columns* (no interruptions occur unless there is a problem with the column or surrounding process units). In this paper we only focus on binary columns, a kind of continuous columns whose feed contains only two components (water and alcohol, for instance). Figure 2 shows a typical equipment for distillation, which often includes a distillation column (indicated by the dashed square in the figure), a reboiler and a condenser.

The *distillation column* (1) consists of several *trays* (2), which allow the simultaneous travel of liquid down the tray and vapor up the tray, allowing mixing of the two phases and therefore equilibrium. The liquid mixture that is to be processed is known as the *feed* (3) and it is introduced usually somewhere near the middle of the column to a tray known as the *feed tray*. The feed tray divides the column into a top (*enriching* or *rectification*) section (4) and a bottom (*stripping*) section (5). The feed flows down the column where it is collected at the bottom in the reboiler. Heat from the *reboiler* (6) vaporizes a portion of the liquid feed, and all vaporous feed travels up the column into rectifying section, while all liquid feed travels down into the stripping section of the column. When the liquid reaches the bottom of the column, it is fed into the reboiler where heat generation causes a portion of liquid to vaporize; when all of the liquid enter-

Fig. 1. Two examples of distillation columns

Fig. 2. Basic scheme of a distillation column

ing from the bottom plate is vaporized, this is called a total reboiler. All vapor produced is returned to the bottom of the column, while any liquid remaining is removed as bottom product or *bottoms* (7).

A similar event occurs at the top of the column. The vapour moves up the column, and as it exits the top of the unit, it is cooled by a *condenser* (8). The condensed liquid is stored in a holding vessel known as the *reflux drum* (9). Some of this liquid is recycled back to the top of the column and this is called the *reflux* (10). The condensed liquid that is removed from the system is known as the top product or *distillate* (11). Thus, there are internal flows of vapour and liquid within the column as well as external flows of feeds and product streams, into and out of the column.

3 McCabe-Thiele's Method

One of the most typical methods to calculate the design parameters of the column is the graphical scheme originally developed by McCabe and Thiele [6]. This is the simplest method to find the number of equilibrium stages for a given distillation process. It should be remarked, however, that it only can be used for systems containing two components. Because of that, we usually omit the component index for the light component, i.e. we write $x = x_1$ (light component) and $x_2 = 1 - x$ (heavy component). On the other hand, McCabe-Thiele's method also requires some additional assumptions. In particular, it is assumed that: (1) the molar overflow is constant, (2) the molal heats of vaporization of the components are roughly the same and (3) heat effects are negligible.

Under these conditions, McCabe-Thiele's method allows us to determine the theoretical number of stages for the separation of a binary mixture and hence, the number of trays required for the distillation column design. The method is also useful to analyze the effects of some column parameters on such a number, as we will show later.

The first step in McCabe-Thiele's method is to plot the vapor-liquid equilibrium data for a component of the binary mixture of composition x_f . To this end, the compositions of liquid and vapor are plotted on the x -axis and the y -axis respectively (see Fig. 3(a)). One method for determining the equilibrium curve is given by:

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

where α is the geometric average relative volatility of the lighter component with respect to the heavier one. In this paper we will consider α as a constant. This assumption holds well for the separation of similar components, for example, for alcohols or for hydrocarbons. However, this is not true for non-ideal mixtures such as azeotropes. The picture of Eq. (1) is known as the *vapor-liquid equilibrium* (VLE) plot (see Fig. 3(a)). Then, the operating lines defining the mass balance relationships between the liquid and vapor phases are drawn as follows: first, we set the desired compositions of the distillate x_d and the bottoms x_b . In the example of Figure 3 they are 0.85 and 0.05, respectively. The next step is to plot the operating line for the rectification section of the column (the part of the column above the feed tray, as shown in Fig. 3(c)). This operating line is given by:

Fig. 3. McCabe-Thiele's method for binary distillation column design: (a)-(h) different steps of the method (see the body text for details)

$$y = \frac{R}{R+1}x + \frac{x_d}{R+1} \quad (2)$$

and hence its slope is $\frac{R}{R+1}$ where $R = \frac{L}{D}$ is called the reflux ratio and is a measure of how much of the material going up the top of the column is returned back to the column as reflux L , the rest being the distillate flow D . Then, we consider the feed line, plotted from the point $(x_d, 0)$ until the straight line $y = x$ and then, depending on the state of the feed, considering different slopes q . For example, $q = 0$ corresponds to saturated vapor (see [7] for details). Finally, the operating line for the stripping section is obtained by tracing a vertical line from the point $(x_b, 0)$ until reaching the diagonal line, and then another line from such a point (x_b, x_b) until the intersection point between the operating line of the rectification section and the feed line, as shown in Figure 3(d).

It is important to remark that the previous scheme describes actually the case of total efficiency. However, in many situations it is more realistic to use of the so-called Murphree's efficiency $E_f \in [0, 1]$. The consequence of this factor is a modification of the original VLE curve. For example, for $E_f = 0.6$ the VLE curve displayed in Figure 3(a) must be replaced by the new VLE curve shown in Figure 3(e).

The next phase of McCabe-Thiele's graphical method is the determination of the number of stages in the distillation process. This is a sequence of similar steps giving rise to a number of "corner" sections, associated with the stages. To understand how they are constructed, let x and y denote the liquid and vapor compositions and the subscripts denote the origin of the flows or compositions. That is, $n - 1$ will mean "from the stage below stage n " while $n + 1$ will mean "from the stage above stage n ". The liquid in stage n and the vapor above it are in equilibrium implying that x_n and y_n lie on the equilibrium curve. Since the vapour is carried to the tray above without changing composition, this is depicted as a horizontal line on the VLE plot. Its intersection with the operating line will give the composition of the liquid on tray $n + 1$ as the operating line defines the material balance on the trays. The composition of the vapour above the $n + 1$ tray is obtained from the intersection of the vertical line from this point to the equilibrium curve. Figure 3(f) shows this process for the third stage (i.e. for $n = 3$). Repeating this sequence back from point (x_d, x_d) until crossing the vertical line at x_b , the diagram of Figure 3(g) is obtained. The calculation of the number of stages reduces simply to count the number of "corners" as shown in 3(g). In our example, we finally obtained a distillation column with 10 trays, where this number also includes the reboiler (see Figure 2).

4 An Illustrative Example

The method described in the previous section has been implemented as a Mathematica package, called `MTBDC.m`, where this acronym stands for *McCabe-Thiele Binary Distillation Column*. This section describes one example of application

of this program to a equimolar (i.e. $x_f = 0.5$) binary mixture whose relative volatility is $\alpha = 4$. Our target is to design a distillation column that obtains a destillate with 85 % of purity (i.e. $x_d = 0.85$) and bottoms with 5 % of purity (i.e. $x_b = 0.05$). The first comand `Reflux[xd,xf,alpha]` determines three values: the reflux, and the liquid and vapor compositions of the more volatile component:

```
In[1]:= Needs["MCBDC"]
In[2]:= Reflux[0.85,0.5,4]
Out[2]:= {1.75,0.2,0.5}
```

Then, the command `OperatingLines[xd,xf,alpha]` is applied to the calculation of the operating lines of the rectification section (given by Eq. 2) and the stripping section, shown in Fig. 3(d). The third step is to apply McCabe-Thiele's method to determine the number of trays of the column as well as the location of the feed tray. To this end, we define the `MTPlot` command, which accepts five different arguments, namely, x_d , x_f , x_b , α and the efficiency E_f (see Section 3 for details). For example, `MTPlot[0.85,0.5,0.05,4,0.6]` returns a sequence of 49 frames corresponding to the different steps of McCabe-Thiele's method. Eight of these frames are displayed in Figure 3.

One of the most outstanding Mathematica features in this work is the possibility to generate QuickTimeTM movies [1]. For example, the different images in Figure 3 correspond to eight frames of a QuickTime movie that reproduces McCabe-Thiele's method in a graphical way. The movie is automatically generated from the `MTPlot` command. Different values of its arguments are associated with different initial mixtures and/or final products. This option is specially valuable for educational and training purposes, as we can obtain a virtually unlimited set of distillation columns in a fast, simple and free-error way.

McCabe-Thiele's method does not allow us to determine all the relevant distillation column parameters and thus, some additional equations must also be considered. The discussion is beyond the scope of this paper and will not be included here. The interested readers are referred to [2,7] for a detailed description on these topics. At this time it is enough to say that a number of different Mathematica commands incorporating these additional equations have been implemented by the authors in the `MTBDC.m` package. For example, if we start with an equimolar mixture of heptane-octane with a relative volatility $\alpha = 2.17$ and efficiency $E_f = 1$ and we wish to obtain a destillate with 98 % of heptane and bottoms with only a 5% of heptane, the column parameters can be determined as:

```
In[3]:= ColumnParameters[0.98,0.05,0.5,2.17,1]
Out[3]:= Number of trays = 14 (rebolier included)
        Number of Feed tray = 9
        Column height = 8.4 meters
        Distance between trays = 0.6 meters
```

Fig. 4. McCabe-Thiele's method for an equimolar heptane-octane mixture with $x_d = 0.98$, $x_f = 0.5$, $x_b = 0.05$ and $\alpha = 2.17$: $E_f = 1$ (above); $E_f = 0.65$ (below)

Figure 4 shows the McCabe-Thiele's diagram of the column for total efficiency $E_f = 1$ (above) and when the efficiency of the process is only a 65 %, that is $E_f = 0.65$ (below). In the first case, the column has only 14 trays and its height

is 8.4 meters, while in the second case the number of trays increases up to 22 and the column height is now 13.2 meters.

5 Conclusions and Further Remarks

In this paper, we describe a Mathematica program for the design of distillation columns for binary mixtures through McCabe-Thiele's method. This program is adequate simulate a virtually unlimited set of distillation columns as well as to analyze the role of the different parameters involved in a very easy way. For example, the simple case of Figure 4 shows how much a single parameter (the efficiency of the distillation process, for instance) can influence the column design, by modifying many relevant parameters such as the number of trays, their location and the height and diameter of the column. We can conclude that the package has a potential from both the industrial and the pedagogical points of view.

All the commands have been implemented in Mathematica version 4 [12]. The symbolic capabilities and the powerful Mathematica functional programming [4] have been extensively used to make the program shorter and more efficient. We finally remark that in the case of multicomponent mixtures, the mathematical representation of the VLE becomes more complex, making necessary to use more complex equations. This is actually our proposal for future work.

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