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Reflections on the use of the Mccabe and Thiele method

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Abstract
This paper reflects on the continuity of teaching the McCabe and Thiele method on chemical engineering courses for understanding the vapour-liquid equilibrium phenomena involved in distillation. Some exercises comparing the results obtained by this method as well as by other accurate analytical methods are presented and solved, as they are taught in ISEL courses. Because of its accuracy and easiness of use, and also because of the fact as this method allows an easy visualisation of the whole operation itself, the McCabe and Thiele method continues to be widespread used and students show a remarkable adherence to it.

Introduction

The issue of June, 1925 of Industrial and Engineering Chemistry published a famous paper entitled "Graphical Design of Fractionating Columns" by W.L. McCabe and E.W. Thiele, of the Massachusetts Institute of Technology [1], described as "A rapid and accurate graphical method (…) for computing the theoretical number of plates required in a given separation of a binary mixture (…)".

Although the precise design of columns for separating binary mixtures of volatile components dates back to a paper by Sorel in 1889 [2], assuming that equilibrium is established between the liquid on each plate and the vapour rising from it, and therefore calculating the enrichment from plate to plate by heat and material balances. This model is applicable to a wide range of continuous, steady state and equilibrium-stage distillation operations, but is somewhat tedious, which resulted in further simplifications made by several authors such as Lewis [3] and Peters [4], among others. Apart from these analytical methods, graphical methods were also introduced by Ponchon [5], Rodebush [6], Savarit [7] and, of course, McCabe and Thiele.

What is striking is the fact that, after the mathematical model of Sorel was published, these other methods were proposed for solving the related equations graphically or algebraically during an 18-year period from 1920 to 1938, prior to the availability of digital computers, which allowed even to solve equations for multicomponent distillation.

Today, the only method from that era that remains in considerable widespread use, still being taught in graduate chemical engineering courses all over the world and described in the major textbooks dealing with unit operations [8], is, in fact, the method of McCabe and Thiele.

The latter method has some attributes that are, and probably will be, responsible for its continuing popularity: it shows clearly the ease or difficulty of each specific separation, as pinched regions can be readily seen, as well as the effect of feed location, in spite of being accurate. Also it can be even applied to more complex problems such as separation of azeotropes, ternary mixtures, etc. Apart from distillation itself, this graphical method has been applied with success to other unit operations such as gaseous absorption and stripping where the basic phenomena involved are basically the same. This method can even be applied to liquid-liquid extraction for constructing auxiliary curves within the application of the Hunter-Nash method [9], and also to the design of multicomponent distillation mixtures.

Calculations on distillation

In order to illustrate this some exercises are currently solved in the classes of Separation Processes as taught in the graduate course of Chemical Engineering of ISEL – Instituto Superior de Engenharia de Lisboa, where from simple examples it is intended to show to the student the easiness and accuracy of the McCabe and Thiele method, particularly when applied to more complex situations other than simple binary distillation.

The following example is particularly useful in order to assess the applicability of the McCabe and Thiele method, especially when compared with other analytical methods, such as Fenske [10] and Kirkbridge [11] methods.

Let us consider the following problem, introduced by Seader and Henley [8]: a 25 mol% mixture of acetone (A) in water (W) is to be separated by distillation at an average pressure of 130 kPa (975 torr), into a distillate containing 95 mol% acetone and a bottoms containing 2 mol% acetone. The infinite-dilution activity coefficients are, respectively:

$$\gamma^{\infty}_{\text{acetone}} = 8.12 \quad \gamma^{\infty}_{\text{water}} = 4.13$$

Using the McCabe and Thiele it is possible to calculate the number of equilibrium stages required. Apart from that let us also calculate the same by using the Fenske equation and then draw conclusions.

Preliminary analysis of thermodynamic data

As the pressure is close to 1 atm, the vapour-liquid equilibrium compositions can be estimated from the modified Raoult's law for ideal gases:

$$K_i = \gamma^{\infty}_{iL} P^s_i / P \qquad \text{Eq. (1)}$$

Vapour pressures can be obtained from Antoine equations and liquid-phase activity coefficients over the entire composition range from fitting the infinite dilution coefficients to the two-constant van Laar equation:

$$\ln \gamma_1 = A^{12} / [1+(x_1A_{12})/(x_2A_{21}]^2 \qquad \text{Eq. (2)}$$

$$\ln \gamma_2 = A_{21} / [1+(x_2A_{21})/(x_1A_{12}]^2 \qquad \text{Eq. (3)}$$

Thus:

$$K_A = y_A/x_A = \gamma_A P^s_i / P \qquad \text{Eq. (4)}$$

and: $K_W = y_W x_W = \gamma_W P^s_W / P$ Eq. (5)

Solving equations (2) and (3) to the activity coefficients:

$$\gamma_A = \exp (A_{AW} / [1+ (x_A A_{WA}/x_W A_{AW})] \qquad \text{Eq. (6)}$$

$$\gamma_W = \exp (A_{WA} / [1+ (x_W A_{AW}/x_A A_{WA})] \qquad \text{Eq. (7)}$$

and, as: $A_{AW} = \ln \gamma^{\infty}_A = \ln (8.12) = 2.094$

$A_{WA} = \ln \gamma^{\infty}_W = \ln (4.13) = 1.418$

Substituting these van Laar coefficients into equations (6) and (7), we obtain:

$$\gamma_A = \exp (2.094 / [1+ (1.477 _{xA} /(1-_{xA})]^2 \qquad \text{Eq. (8)}$$

$$\gamma_W = \exp (1.418 / [1+ (0.6772 (1-_{xA})/_{xA}]^2 \qquad \text{Eq. (9)}$$

Now, we have to consider the correlation between temperature and pressure of the gaseous phase for both substances, which can be obtained from Perry's Chemical Engineers' Handbook [12], as follows:

$\log P^s_A = 7.11714 - 1210.595 / (T+229.664)$ Eq. (10)
$\log P^s_W = 8\text{-}07131 - 1730.630 / (T+233.426)$ Eq. (11)
where: P^s_i is the vapour pressure of component i (torr) and T is the temperature (°C).

Determination of the minimum stages by the Fenske equation

In order to apply the Fenske equation, it is necessary, first, to determine the relative volatilities at the top and at the bottom of the column. Then the average value can be used to compute the Fenske equation.

Bubble point for the distillate composition

The bubble point condition is:

$$\Sigma_i x_{Di} K_i = \Sigma_i x_{Di} (\gamma_i P^s_i / P) = 1 \qquad \text{Eq. (12)}$$

In the distillate, xA = 0.95 and $x_W = 0.05$. From equations (6) and (7):

$\gamma_A = \exp (2.094 / [1+ (0.95x2.094 / 0.05x1.418)]^2 = 1.003$
$\gamma_W = \exp (1.418 / [1+ (0.05x1.418 / 0.95x2.094)]^2 = 3.75$
Then, equation (12) becomes:
$0.95 (1.003 P^s_A/975) + 0.05 (3.75 P^s_W/975) = 1$, where the vapour pressure is expressed in torr.

Now, using equations (10) and (11), by a trial and error calculation, we obtain a distillate temperature of 64 °C. Then, from equations (4) and (5), $\alpha_{A,W} = K_A/K_W = 1.48$

Bubble point for the bottoms composition

In the bottoms $x_A = 0.02$ and $x_W = 0.98$. Again, from equations (6) and (7):
$\gamma_A = \exp (2.094 / [1+ (0.02x2.094 / 0.98x1.418)]^2 = 7.19$
$\gamma_W = \exp (1.418 / [1+ (0.98x1.418 / 0.02x2.094)]^2 = 1.001$
Equation (12) now becomes:
$0.02 (7.19 P^s_A/975) + 0.98 (1.001 P^s_W/975) = 1$, where the vapour pressure is expressed in torr.

Now, using equations (10) and (11), again by a trial and error calculation, we obtain a distillate temperature of 95 °C. Then, from equations (4) and (5), $\alpha_{A,W} = K_A/K_W = 27.7$.

The average volatility is the geometric mean average volatility: $(1.48x27.7)^{1/2} = 6.40$

Calculation of the minimum number of stages

The minimum number of stages can now be computed from the Fenske equation:
$N_{min} = \log [(x_{i}, {}_{N+1}/x_{i,\,1}) / (x_{j,1}/x_{j}, {}_{N+1})] / \log \alpha_{ij}$ Eq (13)
$N_{min} = \log [(x_{Da}/x_{Ba}) / (x_{Bw}/x_{Dw})] / \log \alpha_{A,W} = \log [(0.95/0.02)/(0.98/0.05)]/\log 6.40 = 3.7$

Determination of the minimum stages by the McCabe and Thiele method

In order to apply the McCabe and Thiele method, it is necessary to obtain the y-x equilibrium curve at the operating pressure of the column (975 torr) in terms of acetone molar fractions. This can be obtained by performing the bubble-point calculations, as above, for a set of points in the range of liquid compositions between the distillate and bottoms compositions: for each point, the K-value and the acetone vapour mole fraction are obtained from equation (1). The obtained results are presented on table 1.

Table 1 Data for y-x equilibrium curve

T (°C)	y_A	x_A
107.1	0	0
95.1	0.361	0.02
84.9	0.578	0.05
76.8	0.705	0.1
73.1	0.754	0.15
71.2	0.777	0.2
70.2	0.789	0.25
69.6	0.796	0.3
69.2	0.801	0.35
68.9	0.806	0.4
68.6	0.811	0.45
68.3	0.817	0.5
67.9	0.824	0.55
67.5	0.833	0.6
67.0	0.842	0.65
66.5	0.855	0.7
66.0	0.87	0.75
65.5	0.889	0.8
65.0	0.911	0.85
64.5	0.936	0.9
64.0	0.965	0.95
63.6	1	1

The McCabe and Thiele plot referring these data is shown in figure 1. The equilibrium stages for total reflux are stepped off between the equilibrium curve and the 45° line, which represents the operating line, from the acetone $x_D = 0.95$, down to the acetone $x_B = 0.02$.

From this plot it can easily be seen that there are 5 minimum stages, which is 35% higher than the 3.7 minimum stages that were obtained by the Fenske equation.

However, it should be noted that the Fenske equation is not reliable for highly non-ideal systems, such as this one.

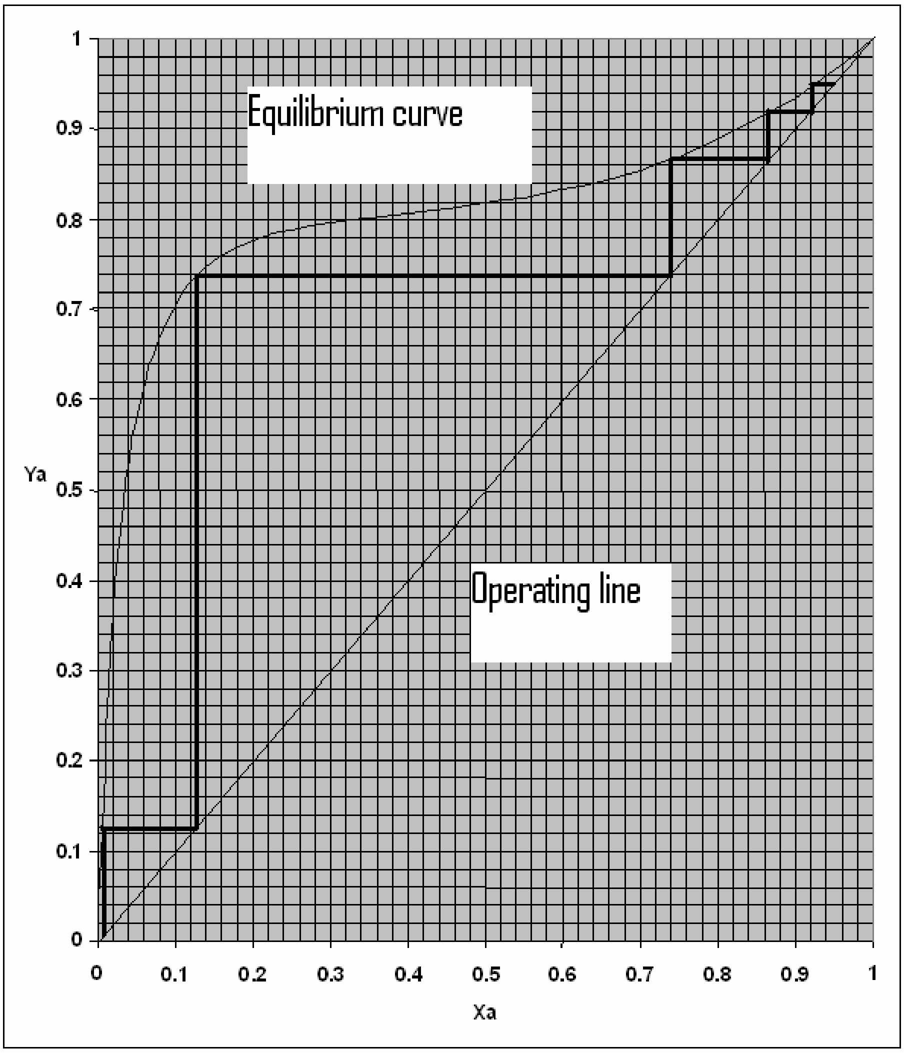

Figure 1 Plot for obtaining equilibrium stages by the McCabe and Thiele method

Apart from that the McCabe and Thiele method presents to the student a clear picture of the whole operation and also allows for some sensitivity analysis as he can analyse quickly the effect of changes on the operational conditions such as feed condition, and the number of stages necessary in order to obtain slightly different x_D or x_B starting from the same point x_F.

In order to assess the full extension of the methods, we, usually proceed with this exercise now to determine the ratio of rectifying to stripping equilibrium stages, as given by the Fenske equation, the Kirkbridge equation and the McCabe and Thiele method.

Then, part 2 of this exercise, consists in determining the ratio of rectifying to stripping stages regarding the same mixture and operational conditions, using the Fenske equation, the Kirkbridge equation and the McCabe and Thiele method.

Fenske equation

The table 2 sums up the composition of the different streams.

Table 2 Composition of feed, distillate and bottoms

Component	z_F	x_D	x_B	$\alpha_{i,\ wi,D}$	$\alpha_{i,\ wi,B}$
Acetone	0.25	0.95	0.02	1.48	27.7
Water	0.75	0.05	0.98	1.00	1.0

For computing the results using the Fenske equation, the relative volatility at feed conditions is also needed: assuming a bubble-point liquid feed, from vapour-liquid data table 1, we obtain:

$\alpha_{i,\ w}$ = [(0.789/0.250)] / [(0.211/0.750)] = 11.2

From the Fenske equation for determining feed-stage location:

$N_R / N_S \approx (N_R)_{min} / (N_S)_{min}$ Eq. (14)

or: $NR / NS = \log [(x_{LK,D}/z_{LK,F}) (z_{HK,F}/x_{HK,D}) \log [(\alpha_B, \alpha_F)^{1/2}] /$

$/ \log [(z_{LK,F}/x_{LK,B}) (x_{HK,B}/Z_{HK,F}) \log [(\alpha_D, \alpha_F)^{1/2}]$ Eq. (15)

Thus:

$N_R / N_S = \log [(0.95/0.25)(0.75/0.05)] \log [(27.7x11.2)^{1/2})] /$

$/ \log [(0.25/0.02)(0.98/0.75)] \log [(1.48x11.2)^{1/2}] = 2.96$

Kirkbridge equation

As the Fenske equation is not reliable except for fairly symmetrical feeds and separations, a reasonably good approximation of optimal feed-stage location can be made by employing the empirical Kirkbridge equation [11]:

$N_R / N_S = [(z_{HK,F}/z_{LK,F}) (x_{LK,B}/x_{HK,D})^2 (B/D)]^{0.206}$ Eq. (16)

By material balances on acetone and water, we get: B/D = 0.753/0.247 = 3.05 and now:

$N_R / N_S = [(0.75/0.25) (0.02/0.05)^2 (3.05)]^{0.206} = 1.08$

McCabe and Thiele method

From the McCabe and Thiele graph shown on figure 1, the total number of minimum stages is 5. The ratio of the number of rectifying stages to stripping stages can also be derived from the graph as:

$N_R / N_S = 4.2/0.8 = 5.25$

In this particular example, the McCabe and Thiele method is the most accurate. The Fenske equation is somewhat better than the Kirkbridge equation, because the latter does not take into account the drastic change in relative volatility occurring from the distillate to the bottom streams, as pointed out by Oliver [13].

Conclusion

This example clearly shows the students that when the assumption of constant molar overflow is valid in each of the two sections of a distillation column, the McCabe and Thiele graphical method is convenient for determining stage and reflux requirements. This method facilitates the visualization of many aspects of distillation and also provides a procedure for locating the optimal feed-stage location. Further examples can be drawn, showing that the McCabe and Thiele method can be extended to handle Murphree stage efficiency [14], multiple feeds, side streams, open steam, as well as the use of reboilers and intercondensers.

From the student's opinions on this ISEL course, it was concluded that the effort required to learn this method is well justified, mainly because it provides an unique tool for solving chemical engineering problems about unit operations dealing with phase equilibrium. It is believed that this fact will provide for the continuity of use of the McCabe and Thiele method in chemical engineering course.

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