Simple New Algorithm for Distillation Column Design

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Separation of a mixture into two or more products through distillation is very common in the process industry. For a given feed mixture and specified product purity requirements, the design of distillation columns typically involves determination of the number of plates, feed-plate location, reflux, and reboil ratio. Preliminary values of these design variables are often determined by trial and error using the McCabe-Thiele method (McCabe and Thiele, 1925). Since distillation is an energy intensive process, it is desirable to determine the values of these design variables corresponding to a minimum in terms of cost of operation. Rigorous simulation and optimization are commonly employed to determine the optimal design.

In this article, a simple new method, which is visual (graphical) and has a similar starting point as the McCabe-Thiele method (that is, use of vapor−liquid data), is proposed for determination of the distillation column design variables. A novel feature of this method is that the determined values of the design variables correspond to a near-optimal (or optimal) solution with respect to cost of operation, without requiring any rigorous simulation or optimization. The new method is based on identification of the largest driving force, defined as the difference in composition between the vapor and liquid, and its relation to feed-plate location. This driving-force concept is similar to the idea of separation power (Seader and Henley, 1998). In its present version, this method is applicable to distillation columns with one feed and two products for binary as well as multicomponent mixtures.

Theoretical Background

Like the McCabe-Thiele method (1925), the starting point is the graphical representation of the vapor−liquid data. However, instead of plotting the vapor composition (y_i) against the liquid composition (x_i), the driving force (F_{Di}) is plotted as a function of liquid (or vapor) composition. F_{Di} is defined as

$$F_{Di} = y_i - x_i = \frac{x_i \alpha_{ij}}{1 + x_i(\alpha_{ij} - 1)} - x_i. \tag{1}$$

Since energy needs to be added or removed to maintain the existence of the vapor and liquid phases, the value of F_{Di} is indirectly related to the energy added or removed. If F_{Di} is large, less energy is involved, while if F_{Di} is small, more energy is involved. A plot of $|F_{Di}|$ vs. x_i for a constant $\alpha_{12} = 3$ is shown in Figure 1. It can be seen that F_{Di} is a concave function with respect to x_i with a well-defined maximum. The BD_y and AD_y lines represent operating lines corresponding to minimum reflux, while BD and AD represent operating lines intersecting on the line $D_y - D_x$ for a reflux greater than the minimum. As $x_i \rightarrow 0$ or 1, $|F_{Di}| \rightarrow 0$. This phenomenon is also observed for other binary mixtures. Figure 2 shows plots of four different types of binary mixtures, with α_{ij} calculated as a function of temperature, pressure, and composition (employing a suitable model). The plots in Figure 2 confirm that the F_{Di} vs. x_i function for a nonazeotropic mixture is

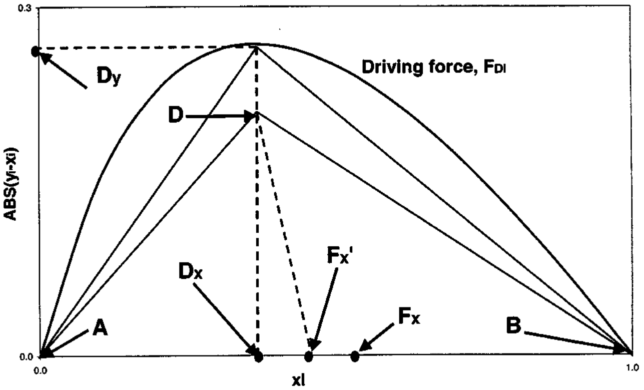

Figure 1. Driving-force-based separation efficiency for constant $\alpha = 3$.

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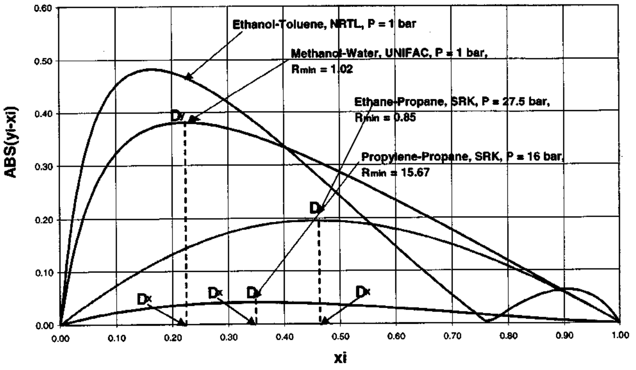

Figure 2. Driving-force-based separation efficiency diagrams for binary mixtures.

All $R_{\min}$ values refer to purity specifications of 99% purity of the light and heavy key components in the top and bottom products, respectively.

concave, while for an azeotropic mixture (for example, ethanol–toluene) there are two concave regions, one on either side of the azeotrope. The value of x_i, where F_{Di} has the maximum value, is obtained by differentiating F_{Di} with respect to x_i. For a constant α_{ij}

$$dF_{Di}/dx_i = \alpha_{ij}/\left(1 - x_i + \alpha_{ij} x_i\right)^2 - 1 = 0. \qquad (2)$$

Since x_i has limits of 0 and 1, only positive values of x_i from Eq. 2 are of interest. Therefore, for constant α_{ij}, $x_i|_{\max}$ corresponding to $F_{Di}|_{\max}$ is obtained from Eq. 2.

$$x_i|_{\max} = \sqrt{(\alpha_{ij} - 1)/(\alpha_{ij} - 1)}\,. \qquad (3)$$

Since α_{ij} is greater than 1 for $F_{Di} > 0$, $x_i|_{\max}$ from Eq. 3 is always positive and less than 1. The locations of $x_i|_{\max}$ and $F_{Di}|_{\max}$ are shown in Figure 1 by the points D_x and D_y, respectively.

According to the new method, if the feed plate is located on the line $D_y - D_x$, the resulting design of the distillation column corresponds to the minimum (or close to minimum) with respect to cost of operation. The basis for this hypothesis is explained below for the case of constant α_{ij}.

Consider the points A and B (see Figure 1) representing the specified compositions for the distillate and bottom products, respectively. According to the new method, the slopes of the operating lines for the rectifying and stripping sections are determined so that they intersect on the line $D_y - D_x$. Intersection at point D_y corresponds to minimum reflux ratio for a saturated liquid feed of composition D_x. For total reflux, the two operating lines have the same slope (in this case, zero) as in the McCabe-Thiele method. Any feed (F_x' in Figure 1) to the right of D_x and between $D_x - F_x$ indicates an unsaturated feed, while F_x (see Figure 1) indicates the saturated vapor feed. The location of F_x on the x-axis is determined from the vapor–liquid relation,

$$F_x = D_x \alpha_{ij}/\left[1 + D_x(\alpha_{ij} - 1)\right]. \qquad (4)$$

A point of intersection for the operating lines to the left of $D_y - D_x$ means a higher reflux ratio but a lower reboil ratio, while a point of intersection to the right of $D_y - D_x$ means a lower reflux ratio but a higher reboil ratio. The sum of the angles defined by BAD_y and D_yBA is the largest compared to all other pinch conditions (the operating lines intersecting on the F_{Di} vs. x_i surface). Therefore, this operating point signifies the lowest cost of operation and the largest total driving force, since larger driving force involves lower amounts of energy. Since the actual reflux ratio (RR) is proportional to the minimum reflux ratio, the locus of points given by $D_y - D_x$ contains the locus of the points of intersections for the operating lines corresponding to the largest actual driving force with $RR_{\min} < RR < RR_{\text{total}}$. This phenomenon also appears to be true if α_{ij} is not constant (as shown in the application examples). Note that with the location of the feed point on $D_y - D_x$ known, the corresponding reflux and reboil ratios and product composition (or number of plates) can easily be determined.

Step-by-step algorithm

Consider the following design problem: given a mixture to be separated into two products in a distillation column with the number of plates (N). What is the optimal (with respect to cost of operation) feed-plate location and the corresponding reflux ratio for different product purity specifications? The solution involves the following steps.

1. Generate or retrieve from a database the vapor–liquid data for the binary system. For a multicomponent system, select the two key components to define the "split" and use them as the binary (key) mixture.
2. Compute F_{Di} using Eq. 1 and plot F_{Di} as a function of x_i, where $i =$ light key component.
3. Identify the points D_y and D_x (graphically or using Eq. 3).
4. For a given N, determine the feed plate location (NF) from $NF = (1 - D_x)N$, where the plates are counted from the top of the column.

In case of an azeotrope, rescale the x-axis and locate the point D_x as the relative distance between the two points on each side of D_x where the driving force is 0 (A and B). The two points are the azeotrope and the top/bottom product.

The preceding algorithm, it can be noted, is very simple and needs very few calculations. It is also valid for any value of N where the specified separation is feasible. As just shown, the value of NF is valid for all (feasible) product purity specifications. Note that the expression in step 4 of the algorithm locates the feed plate in a distillation column at the relative position corresponding to the maximum driving force in the column.

Normally, with the values of N, NF, product purity, and feed condition specified, the design of a distillation column can be verified through rigorous simulation, or the design can be further investigated in terms of control and operation. For the simulation model, however, it is a good idea to have estimates for the reflux ratio (since it will be calculated) and guarantee that the desired separation is feasible. Therefore, values of reflux ratios are needed to start the validation-related simulations. For specified product purities, the following alternative steps are employed for determination of NF, N, reflux, and reboil (RB) ratios.

5. If the product specifications are given, locate points A and B. Determine the slopes of the lines AD_y and BD_y. Determine the corresponding $RR_{\min}$ and $RB_{\min}$.

6. Choose a value of $C = RR/RR_{\min}$ to locate the point of intersection, D. Draw the operating lines for the rectifying and stripping sections and determine the number of plates in the same way as in the McCabe-Thiele method.

Application Examples

The preceding method has been tested with many binary and multicomponent mixtures, and only three such test examples are highlighted here. The objective of these examples is to show that the minimum (or near-minimum) energy consumption corresponds to a design based on NF located on the line $D_y - D_x$. In each case, an appropriate property model (see Figure 2) has been used to determine the driving force as a function of composition, and the design has been verified through rigorous simulation with the steady-state distillation model in PRO/II (1994). For all simulations, the energy consumption has been calculated for the following specified variables, N, NF, A, B, and feed condition. The simulation program also calculated the reflux ratio using the driving-force-based calculated value as initial estimate. Therefore, if the rigorous simulation reflux ratio is between $RR_{\min}$ and RR_{Total}, the operating lines must intersect at the specified NF. Also, any NF to the right or left of the $D_x - D_y$ line gives a larger reflux ratio or reboil ratio, respectively. A sample of the results is given in this R&D note. Detailed results for all the test examples can be obtained from the authors.

Example 1: Simple separation (methanol-water)

For this example, the driving-force diagram as a function of composition is shown in Figure 2. This is an easy separation with α_{ij} varying between 2.5 and 7.7, while $F_{D1}|_{\max}$ is given by $D_y = 0.38$ at $D_x = 0.22$. The optimum feed location with the Kirkbride equation (as defined by Seader and Henley, 1998) is at $D_x = 0.5$ for an equimolar feed composition, which corresponds to an increase in the energy consumption of 22% compared to the optimal location found by the new algorithm. In Figure 3a, plots of the calculated energy consumption as a function of feed-plate location for various feed compositions and product purity are shown for a fixed number of plates. It can be noted that in each case, NF located on the line $D_y - D_x$ corresponds to the minimum (or near-minimum) energy consumption. In the case of equimolar feed and $NF = 17$, rigorous simulation gave $RR = 3.13$, which is greater than $RR_{\min} = 1.02$ (see Figure 2). The feed to the column was saturated liquid at column pressure = 1 bar.

Example 2: Difficult separation (propylene-propane)

This is a difficult separation, with α_{ij} varying between 1.09 and 1.33. Compared to Example 1, the maximum value of F_{Di} is significantly smaller, $D_y = 0.04$ at $D_x = 0.35$. This means that more plates and energy are needed to perform the desired separation. The plot of the driving force as a function of composition is shown in Figure 2. In Figure 3b, plots of calculated energy consumption as a function of feed-plate location for various feed compositions and product purity are shown for a fixed number of plates. It can be noted that in each case, the design based on the driving force corresponds to the minimum with respect to energy consumption. The Kirkbride equation predicts the feed location at $D_x = 0.5$ for equimolar feed, which corresponds to an increase in the energy consumption of 35% compared to the optimal location found by the new algorithm. With equimolar feed and $NF = 115$, rigorous simulation gave $RR = 20.80$, which is greater than $RR_{\min} = 15.67$ (see Figure 2). The feed, in this case, was saturated liquid at column pressure = 16 bar.

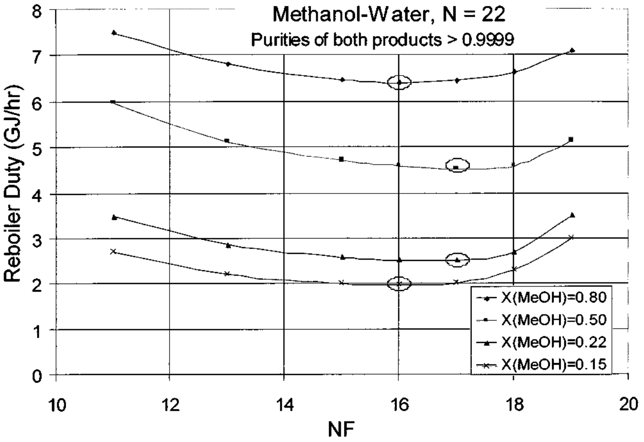

Figure 3a. Heat duties as function of feed location for example 1.

The circled points indicate the optimal feed location.

Example 3: Multicomponent separation

This example, involving the design of a deethanizer column, has been taken from Seader and Henley (1998). Ethane and propane are the key components for a deethanizer column, and the driving force is computed as a function of composition (also shown in Figure 2) for this pair of components. Here, $F_{Di}|_{\max}$ is given by $D_y = 0.19$ at $D_x = 0.48$. Although the Kirkbride equation predicts $D_x = 0.41$, the difference in energy consumption is negligible, since the driving force is relatively large and N is relatively small. Figure 3c shows the

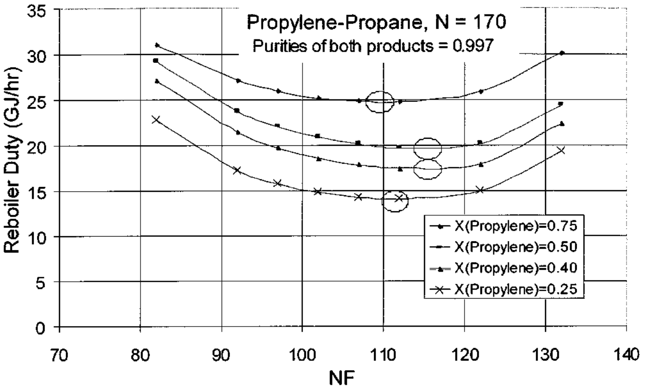

Figure 3b. Heat duties as function of feed location for example 2.

The circled points indicate the optimal feed location.

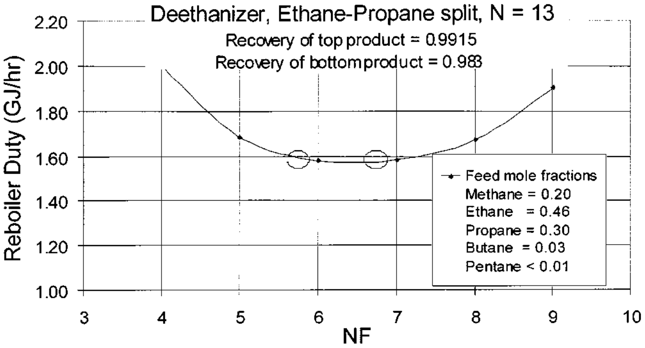

Figure 3c. Heat duties as function of feed location for example 3.

The circled points indicate the optimal feed location.

plot of calculated energy consumption as a function of feed location for a given feed composition and recovery of the key components. Again, in all cases, the minimum energy corresponds to the design with respect to the driving force. For the feed composition given in Figure 3c and $NF = 6$, rigorous simulation gave $RR = 1.10$, which is greater than $RR_{\min} = 0.85$ (see Figure 2). The feed in this case was saturated liquid at column pressure = 27.5 bar.

Conclusion

A simple, visual method for the preliminary design of conventional distillation columns has been proposed and validated with rigorous simulation and optimization studies. Even though a property model has been used to generate the vapor–liquid data, in principal, experimental data could also have been used. Using the same property model in rigorous simulation, however, provided a consistent basis for comparison of results. The validation results confirm that the preliminary design also correspond to an optimal (or near-optimal) solution with respect to the cost of operation as a function of energy consumption. Considering that only a few simple calculations are needed to obtain a design that is close to the optimal, the method has the potential to play a major role in design and analysis of distillation columns and in the integration of synthesis, design, and operation. Although not fully tested, the method also appears to be applicable to rate-based processes as well as multifeed- and/or solvent-based distillation operations. Current work is extending the method to applications in different types of separation processes and configuration of the separation flow sheet, in addition to comprehensive tests of applicability in rate-based processes, complex distillation columns, and solvent-based distillation (azeotropic/extractive distillation).

Notation

A = product purity of light key component
B = product purity of heavy key component
D_x = point on the x-axis corresponding to $F_{Di}|_{\max}$
D_y = point on the y-axis corresponding to $F_{Di}|_{\max}$
X = mol fraction of feed mixture
α_{ij} = relative volatility of component i with respect to component j

Literature Cited

McCabe, W. L. and E. W. Thiele, "Graphical Design of Fractionating Columns," *Ind. Eng. Chem.*, **17**, 605 (1925).

PRO/II User's Guide, Simulation Sciences Inc., Brea, CA (1994).

Seader, J. D., and E. J. Henley, *Separation Process Principles*, Wiley, New York (1998).

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