Multicomponent Distillation

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Distillation columns can be used to separate mixtures of more than two components with the following restrictions:

- If the column has only two products, distillate and bottoms, only two product purities or recoveries can and must be specified. For each additional product stream (called *side products*) one more specification is required.
- The McCabe-Thiele graphical design method is not useful to estimate the number of required stages.

In these notes we will introduce a short-cut method to estimate the reflux ratio and number of stages, known as the Fenske-Underwood-Gilliland method, and will briefly outline how process simulators solve the rigorous distillation models.

1 Column Specifications

The total number of specifications associated with a distillation column with two product streams is C + 6, where C is the number of components in the feed. This includes the specifications required to define the feed to the column, which are C + 1:

- C 1 component mole or mass fractions
- The feed rate
- The feed enthalpy.

Alternatively the flow of each component (*C* flows) and the enthalpy can be specified. The enthalpy can be specified directly or by the following two parameters:

- > The feed temperature and pressure (if the feed is a subcooled liquid or a superheated vapor)
- > The feed temperature or pressure and
 - o Specification that it is a saturated liquid or vapor
 - o The fraction vaporized.

If the column has more than one feed stream each feed stream requires C + 1 specifications to be defined.

This leaves five more specifications to define the column design problem. These are:

- > The column pressure (or pressure profile). The pressure is required to establish the equilibrium relationships.
- > Two product purity or component recovery specifications.
- > The reflux ratio.
- > The specification that the feed be located at its optimum location (see notes on Binary Distillation Design).

The pressure profile is usually specified as either a constant pressure or as the condenser and reboiler pressures assuming a linear profile.

1.1 Key Components and Sequencing Columns

Since in a multicomponent column there are more than two components and only two component purity or recovery specifications, two of the components from the mixture must be selected; these are known as the *key components* and are the components on which the specifications are based. The lighter of the two components is called the *light key* (LK) and the heavier

is the *heavy key* (*HK*). The selection of these two components defines the way the feed mixture is *cut*; that is, the way the mixture is separated into the two product streams. Obviously, most of the light key will go to the distillate and most of the heavy key will go to the bottoms. What happens to the other components? Common assumptions in solving the mass balances on the column are:

- All of the components that are lighter than the light key (*LLK*) go to the distillate.
- All of the components heavier than the heavy key (*HHK*) go to the bottoms.

For example, suppose that we have five components A, B, C, D and E, listed in order of increasing normal boiling points. Figure 1 shows how the components separate if C is selected as the light key and D is the heavy key. The figure shows that components A, B and C go to the distillate and components D and E go to the bottom.



Figure 1. Cutting a 5-component mixture into two products

In the example of Fig. 1 components A and B are lighter than the light key (LLK) and component E is heavier than the heavy key (HHK). Now a small amount of the heavy key D must go to the distillate and a small amount of the light key C must go to the bottoms. How much are the small amounts depends on the product specifications, which are based on the keys, C and D.

Following the same example, how many distillation columns are needed to separate the five components into five streams each containing one of the components? Four is the correct answer, but how should they be sequenced? Figure 2 shows two possible ways to do the sequencing. Note that the sequencing depends on the selection of the light and heavy keys for each column.



Figure 2. Two ways to sequence distillation columns to completely separate five components. There are 12 other ways.

The following are some rules of thumb to help in sequencing distillation columns:

- Remove toxic or corrosive components first to prevent the spread of toxic components or so that only the first one or two columns need to be of corrosion resistant materials.
- Favor equimolal splits to keep the molar feed rates to the following columns smaller.
- Remove the most plentiful component first for the same reason.

- Keep difficult separations for last so that the feed rate to the column is smaller.
- Remove products and recycle streams as distillates to prevent contamination with tars that may form in the bottom of the column.

It is very important to always list the components in order of decreasing volatility, that is, the most volatile component at the top of the list followed by the next volatile component and so on with the heaviest component at the bottom. You must do this always.

2 Over-all Balances

As with a binary distillation column, the first step is to carry out the over-all mole balances on the column to determine the compositions of the product streams. With flows and С two product streams and the feed rate components, and composition specified, there are C independent mole balances and 2C unknowns, two product rates and 2(C - 1) product mole fractions. We have therefore C more unknowns than equations, but... there are only the two key component specifications. This is why we must assume that all of the lighter-than-light-key (LLK) components go to the distillate and all of the heavierthan-heavy-key (HHK) components go to the bottoms product. This gives us C - 2 zero compositions (the LLK components in the bottom and HHK components in the distillate) and we can solve the material balances. This is best demonstrated with an example.

Example 1. Over-all Balances on the Distillation of a Mixture of Hydrocarbons

A mixture at the rate of 200 kmole/hr is to be separated by distillation. The feed contains 10 mole% propane, 45 mole% n-butane, 40 mole% n-pentane and the balance n-hexane. It is desired to obtain a distillate stream containing no more than 4 mole% n-pentane and a bottoms stream containing no more than 2 mole% n-butane. Determine the flows and compositions of the distillate and bottoms product and the recoveries of the key components.



As the specifications are given on n-butane and npentane, these are respectively the light and heavy keys. So the propane is the LLK and all goes to the distillate, so:

$$x_{BC3} = 0$$

The n-hexane is the HHK, so:

 $x_{DC6} = 0$

With four components we have four independent balances:

Total balance: F = D + B = 200 kmole/hr B = 200 - D

Component balances: $Fx_{Fi} = Dx_{Di} + Bx_{Bi}$

Propane: $200(0.10) = Dx_{DC3} + B(0) = 20 \text{ kmole/hr}$ n-butane: $200(0.45) = Dx_{DC4} + (200 - D)0.02 = 90 \text{ kmole/hr}$ n-pentane: $200(0.40) = D(0.04) + (200 - D)x_{BC5} = 80 \text{ kmole/hr}$ Sum of $x_{Di} = 1$: $x_{DC3} + x_{DC4} + x_{DC5} + x_{DC6} = 1.0$ $x_{DC4} = 1.0 - x_{DC3} - 0.04 - 0 = 0.96 - x_{DC3}$ Substitute into n-butane balance: $D(0.96 - x_{DC3}) + (200 - D)0.02 = 90 \text{ kmole/hr}$ $D(0.96 - 0.02) = 90 + Dx_{DC3} - 200(0.02)$

Substitute propane balance: 0.94D = 90 + 20 - 4 = 106 kmole/hr D = 106/0.94 = 112.8 kmole/hr B = 200 - 112.8 = 87.2 kmole/hr n-hexane balance: $200(0.05) = D(0) + (200 - D) x_{BC6} = 10$ kmole/hr $x_{BC6} = 10/87.2 = 0.115$ $x_{BC5} = 1.0 - 0 - 0.02 - 0.115 = 0.865$ Compositions: Distillate Bottoms Propane: 20/112.8 = 0.177 0 n-butane: 0.96 - 0.177 = 0.783 0.020

n-pentane: 0.040 0.865 n-hexane: 0 0.115 Recoveries: n-butane in distillate: 0.783(112.8)/90 = 0.98

n-pentane in bottoms: 0.865(87.2)/80 = 0.94

In the preceding example the n-butane (LK) composition is specified in the bottoms product and the n-pentane (HK) composition is specified in the distillate. These are small numbers and are specified this way so that the recoveries of the key components are high. Notice that there is no convenient way to specify the composition of the LK in the distillate (0.783) or of the heavy key in the bottoms (0.865) to ensure the recoveries to be high. This is why

you must always specify the light key composition in the bottoms product and the heavy key composition in the distillate!

Having calculated the flows and compositions of the products, we are now ready to design the column by determining the liquid and vapor flows and the required number of stages. We will do this by the short-cut design method.

3 Short-Cut Distillation Design Method

The short-cut distillation design method is carried out in three steps:

1. Determine the minimum number of equilibrium stages at total reflux using the Fenske equation.

- 2. Determine the minimum reflux ratio using the Underwood equation.
- 3. Determine the number of equilibrium stages at a specified reflux ratio, or the reflux ratio at a specified number of equilibrium stages using the Gilliland correlation.

These will be presented next.

3.1 Minimum Number of Stages by Fenske

In the Binary Distillation Design notes we learned that at total reflux, D = 0, B = 0:

- The required number of equilibrium stages is minimum,
- The operating lines become $y_{n+1} = x_n$.

Assuming that the relative volatility α_{ij} of component *i* to component *j* is constant, a formula can be derived to calculate the minimum number of stages at total reflux. This formula is known as the *Fenske* equation. The following is the derivation.

A: Equilibrium relation:
$$\alpha_{ij} = \frac{y_{in}x_{jn}}{x_{in}y_{jn}}$$
 or $\frac{y_{in}}{y_{jn}} = \alpha_{ij}\frac{x_{in}}{x_{jn}}$

B: Operating line: $y_{n+1} = x_n$

C: Combine A and B: $\frac{x_{in}}{x_{jn}} = \frac{y_{i,n+1}}{y_{j,n+1}} = \alpha_{ij} \frac{x_{i,n+1}}{x_{j,n+1}}$

D: At the top of the column: $y_1 = x_D$

E: From C:
$$\frac{y_{i1}}{y_{j1}} = \frac{x_{iD}}{x_{jD}} = \alpha_{ij} \frac{x_{i1}}{x_{j1}} = \alpha_{ij}^2 \frac{x_{i2}}{x_{j2}} = \dots = \alpha_{ij}^{N_{min}} \frac{x_{i,N_{min}}}{x_{j,N_{min}}}$$

F: At the bottom of the column: $x_{N_{min}} = x_B$

G: Substitute F in E:
$$\frac{x_{iD}}{x_{jD}} = \alpha_{ij}^{N_{min}} \frac{x_{iB}}{x_{jB}}$$
 or $\alpha_{ij}^{N_{min}} = \frac{x_{iD}x_{jB}}{x_{jD}x_{iB}}$

H: Take logarithm:
$$N_{\min}\ln(\alpha_{ij}) = \ln\left(\frac{x_{iD}x_{jB}}{x_{jD}x_{iB}}\right)$$

Solve for N_{\min} to obtain the Fenske equation:

$$N_{\min} = \frac{\ln\left(\frac{x_{iD}x_{jB}}{x_{jD}x_{iB}}\right)}{\ln(\alpha_{ij})} \quad (1)$$

The derivation is presented here to show that there is no "- 1" on the equation as most textbooks and handbooks show. The "- 1" is supposedly added to account for a partial reboiler which is not possible because at total reflux both the condenser and the reboiler must be total.

The Fenske equation applies to any two components in the multicomponent mixture, but to calculate the minimum number of stages we must use the two key components. Why? Because the product purity specifications are given on the key components. Once the minimum number of stages is determined, the equation can be used to estimate the compositions of the non-key components in the bottoms and distillate products, the ones assumed to be zero in the mass balances, at total reflux.

Equation (1) shows that the minimum number of stages depends only on the product compositions and the relative volatility of the two key components, and independent of the feed composition and enthalpy, as is the case with binary columns.

When the relative volatility is only approximately constant the geometric average of the values at the top and bottom of the column can be used:

$$\alpha_{ij,avg} = \sqrt{\alpha_{ij,top} \alpha_{ij,bot}} \tag{2}$$

Note that the relative volatilities at the top and bottom are for the same pair of components, not for a different pair.

Example 2. Minimum Number of Stages for a Mixture of Hydrocarbons

The relative volatilities for the components of Example 1 are given at the top and bottom of the column in the table below, along with the results for the specifications of Example 1. Determine the minimum number of equilibrium stages using the Fenske equation. Determine also the compositions of the non-key components at total reflux.

	Component	хF	x _D	X _B	α , top	α , bot
	propane	0.10	0.177	0.000	6.775	11.100
LK	n-butane	0.45	0.783	0.020	2.460	3.172
ΗК	n-pentane	0.40	0.040	0.865	1.000	1.000
	n-hexane	0.05	0.000	0.115	0.422	0.330
	Total	1.00	1.00	1.00		

Note that the relative volatilities are calculated relative to the heavy key, n-pentane.

Solution: Compute the average relative volatilities:

Propane: $\alpha_{13} = \sqrt{(6.775)(11.100)} = 8.671$

n-butane: $\alpha_{23} = \sqrt{(2.460)(3.172)} = 2.793$

n-hexane: $\alpha_{43} = \sqrt{(0.422)(0.330)} = 0.373$

Minimum number of stages:
$$N_{\min} = \frac{\ln\left(\frac{x_{D2}x_{B3}}{x_{D3}x_{B2}}\right)}{\ln(\alpha_{23})} = \frac{\ln\left(\frac{(0.783)(0.865)}{(0.020)(0.040)}\right)}{\ln(2.793)} = 6.6$$

To obtain the compositions of the non-key components at total reflux we apply the Fenske equation to those components:

Propane (LLK):
$$N_{\min} = \frac{\ln\left(\frac{x_{D1}x_{B3}}{x_{D3}x_{B1}}\right)}{\ln(\alpha_{13})} = \frac{\ln\left(\frac{(0.117)(0.865)}{0.020 \ x_{B1}}\right)}{\ln(8.671)} = 6.6$$

$$x_{B1} = \frac{(0.117)(0.865)}{0.020} 8.671^{-6.6} = 3.2 \times 10^{-6}$$

n-hexane (HHK):
$$N_{\min} = \frac{\ln\left(\frac{x_{D4}x_{B3}}{x_{D3}x_{B4}}\right)}{\ln(\alpha_{43})} = \frac{\ln\left(\frac{x_{D4}(0.865)}{0.020\ 0.115}\right)}{\ln(0.373)} = 6.6$$

$$x_{D4} = \frac{(0.020)(0.115)}{0.865} 0.373^{6.6} = 2.0 \times 10^{-4}$$

Both of these mole fractions were assumed to be zero in the mass balances of Example 1. They are small enough so that the mass balance results are not affected.

It is important to realize that, because design calculations involve approximations such as these, the results are only accurate to at most three significant digits. This is why you must not report your results to more than three digits.

3.2 Minimum Reflux Ratio—The Underwood Equation

The minimum reflux ratio, as with binary distillation columns, depends on the enthalpy and composition of the feed, the relative volatilities (equilibrium relations) and the distillate composition. The Underwood equation provides a quick way to estimate the minimum reflux ratio; it requires two steps.

1. Determine the value of \emptyset that satisfies the relation:

$$1-q = \sum rac{lpha_i x_{Fi}}{lpha_i - arnothing}$$
 (3)

2. Use the value of \emptyset to calculate the minimum reflux ratio:

$$R_{Dm} = \sum \frac{\alpha_i x_{Di}}{\alpha_i - \emptyset} - 1 \qquad (4)$$

Where
$$\alpha_i$$
 = relative volatility of component *i*
 q = enthalpy condition parameter of the feed
 x_{Fi} = mole fraction of component *i* in the feed
 x_{Di} = mole fraction of component *i* in the distillate
 R_{Dm} = minimum reflux ratio

The enthalpy parameter q is presented in detail in the Binary Distillation Design notes.

Equation (3) must be solved iteratively. The value of \emptyset can be determined with an appropriate calculator, a workbook or a program such as MathCad or MATLAB. When these are not available the Secant method can be used (see the Flash Distillation notes). However, in this case the iterative solution presents a particular problem, regardless of the solution method used. For a system with *C* components Eq. (3) is a polynomial of degree *C* with *C* different roots, but only one of those roots is valid for use in Eq. (4). How to ensure to obtain the correct value of \emptyset ? By starting the iteration with a value of \emptyset which is between the relative volatilities of the two key components. When this is done the resulting value will be between the two relative volatilities and this is the valid root to use in Eq. (4).

Example 3. Minimum Reflux Ratio for a Mixture of Hydrocarbons

For the conditions of Example 1 determine the minimum reflux ratio. The feed enters the column 40% vaporized, by mole, at the conditions of the feed.

Solution. The average relative volatilities were determined in Example 2. As q is the molar fraction of the feed that is liquid,

$$q = 1 - 0.40 = 0.60$$

Equation 3 to solve for \emptyset :

$$1 - 0.60 = \frac{8.671(0.10)}{8.671 - \emptyset} + \frac{2.793(0.45)}{2.793 - \emptyset} + \frac{1.0(0.40)}{1.0 - \emptyset} + \frac{0.373(0.05)}{0.373 - \emptyset}$$

Secant iteration. The value of \emptyset is between 1.0 and 2.793.

First guess:

$$\emptyset_1 = 2.0 \qquad e_1 = -0.40 + \frac{8.671(0.10)}{8.671-2.0} + \frac{2.793(0.45)}{2.793-2.0} + \frac{1.0(0.40)}{1.0-2.0} + \frac{0.373(0.05)}{0.373-2.0} = 0.903$$
$$\emptyset_2 = 1.5 \qquad e_2 = -0.40 + \frac{8.671(0.10)}{8.671-1.5} + \frac{2.793(0.45)}{2.793-1.5} + \frac{1.0(0.40)}{1.0-1.5} + \frac{0.373(0.05)}{0.373-1.5} = -0.124$$

Secant: $\emptyset_3 = \emptyset_2 - e_2 \frac{\emptyset_2 - \emptyset_1}{e_2 - e_1} = 1.5 - (-0.124) \frac{1.5 - 2.0}{-0.124 - 0.903} = 1.560$ $e_3 = 0.011$

$$\emptyset_4 = 1.560 - (0.011) \frac{1.560 - 1.50}{0.011 - (-0.124)} = 1.555$$
 $e_4 = 0.0006$

The minimum reflux ratio from Eq. (4) with $\emptyset = 1.555$:

$$R_{Dm} = \frac{8.671(0.117)}{8.671 - 1.555} + \frac{2.793(0.783)}{2.793 - 1.555} + \frac{1.0(0.040)}{1.0 - 1.555} + \frac{0.373(0.)}{0.373 - 1.555} - 1 = 0.837$$

In this example the Secant method converges within four iterations.

3.3 Number of Equilibrium Stages—Gilliland Correlation

With the minimum number of stages at total reflux and the minimum reflux ratio, the Gilliland correlation allows the calculation of the required number of equilibrium stages at a specified reflux ratio, or the reflux ratio required for a specified number of equilibrium stages. The original correlation was graphical, shown in Fig. 3.



Figure 3. Gilliland Correlation

The correlation has been converted to the following formula for ease of programming:

$$\frac{N-N_{\min}}{N+1} = 1 - e^{\left(\frac{1+54.4X}{11+117.2X}\right)\frac{X-1}{\sqrt{X}}}$$
(5)

Where
$$X = \frac{R_D - R_{Dm}}{R_D + 1}$$

N = number of equilibrium stages

 N_{\min} = minimum number of stages at total reflux R_D = reflux ratio R_{Dm} = minimum reflux ratio

3.4 Optimum Location of the Feed Tray

The optimum location of the feed stage may be estimated by the Kirkbride equation:

$$\frac{N_R}{N-N_R} = \left[\left(\frac{x_{F,HK}}{x_{F,LK}} \right) \left(\frac{x_{B,LK}}{x_{D,HK}} \right) \frac{B}{D} \right]^{0.206} \tag{6}$$

Where N_R = number of stages above the feed tray, N = number of equilibrium stages B = bottoms product molar rate D = distillate molar rate $x_{F,HK}$, $x_{F,LK}$ = mole fractions of the keys in the feed $x_{B,LK}$ = mole fraction of the light key in the bottoms $x_{D,HK}$ = mole fraction of the heavy key in the distillate

Equation 6 does not provide good estimates of the optimum feed tray location when the relative volatility of the key components

differs significantly from the top to the bottom of the column, or when they form an azeotrope.

Example 4. Number of Equilibrium Stages for Hydrocarbon mixture

Determine the number of actual trays required for the column of Example 1 at a reflux ratio of 1.2 times the minimum ratio and for an over-all column efficiency of 50%. Assume the column has a total condenser and a partial reboiler. Determine also the optimum location of the feed tray.

Solution. The minimum number of stages was calculated in Example 2 and the minimum reflux ratio in Example 3.

$$N_{\min} = 6.6$$
 $R_{Dm} = 0.837$

Reflux ratio: $R_D = 1.2(0.837) = 1.004$

$$\frac{R_D - R_{Dm}}{R_D + 1} = \frac{1.004 - 0.837}{1.004 + 1} = 0.0835$$

From Fig. 3:
$$\frac{N-N_{min}}{N+1} = 0.57$$
 $N = \frac{6.6+0.57}{1-0.57} = 16.7$

Assuming the partial reboiler is an equilibrium stage, the number of actual trays required for 50% over-all efficiency is:

$$N_a = (16.7 - 1)/0.50 = 31.4$$
 or 32 actual trays.

The Gilliland correlation can also be used to estimate the reflux ratio required for a specified number of equilibrium stages.

Optimum feed tray location:

$$\frac{N_R}{N - N_R} = \left[\left(\frac{0.40}{0.45} \right) \left(\frac{0.040}{0.020} \right) \frac{112.8}{87.2} \right]^{0.206} = 1.19$$

$$N_R = N/(1 + 1.19) = 16.7/2.29 = 7.3$$

So, 7.3 stages above the feed and 9.4 below. In real trays (50% efficiency):

Above the feed tray: 7.3/0.50 = 14.6 or 15 trays Below the feed tray: (9.4 - 1)/0.50 = 16.8 or 17 trays

We subtracted one stage from the bottom to account for the partial reboiler.

4 Rigorous Distillation Models

The method presented in the preceding section, sometimes known as the Fenske-Underwood-Gilliland method, is used by process simulators to estimate the number of equilibrium stages at a specified reflux ratio in models also known as *Short-Cut Distillation Models*. Simulators also provide rigorous distillation models that solve the mass and enthalpy balances and equilibrium relationships on each tray. We will briefly present here the equations involved to give an idea of the complexity of the solution procedure.

It is important to understand that the rigorous method is a *rating* method rather than a *design* method. For the rigorous method, instead of specifying the reflux ratio we must specify the number of equilibrium stages and the location of the feed

tray. In other words, the method is designed to rate a proposed column. The five specifications required to solve the rigorous model are:

- 1. The number of equilibrium stages
- 2. The location of the feed stage
- 3. The pressure profile
- 4. Either the reflux or boil-up ratio, the distillate purity or the light key component recovery
- 5. Either the distillate or bottoms product flow, the bottoms product purity or the heavy key component recovery.

Minimum reflux and minimum number of trays have no meaning in the rigorous method.



Figure 4. Schematic of a Tray in a Distillation Column

The rigorous model calculations are performed on each tray. Consider the tray sketched in Fig. 4. A total molar balance results in:

$$L_{k-1} + V_{k+1} = L_k + V_k \tag{7}$$

1 eqn., 2 unks. $[L_k, V_k]$

Where L and V are the molar rates of the liquid and vapor streams (kgmole/hr), respectively, and the subscript k refers to the tray number. Next we write component molar balances for each of the components minus one:

$$L_{k-1}x_{i,k-1} + V_{k+1}y_{i,k+1} = L_k x_{i,k} + V_k y_{i,k}$$
(8)

C eqns.,
$$2C + 2$$
 unks. $[x_{i,k}, y_{i,k}]$

Where x and y are the component mole fractions in the liquid and vapor streams, respectively. The total unknowns include all C components, so we can write:

$$\sum_{i=1}^{C} x_{i,k} = 1 \qquad \sum_{i=1}^{C} y_{i,k} = 1$$
(9)

C + 2 eqns., 2C + 2 unks.

Assuming the tray is an equilibrium stage, the mole fractions are related by:

$$y_{ik} = K_i(T_k, P, x_{ik}) x_{ik}$$
(10)

2C + 2 eqns., 2C + 3 unks. $[T_k]$

Where T_k is the temperature on the tray (K) and P is the pressure (kPa). In counting unknowns we have considered that the K-factor is calculated by the simulator from the specified thermodynamic model, and the pressure is either specified constant or as linearly varying between the specified condenser and reboiler temperatures. Finally an enthalpy balance completes the model of the tray:

$$L_{k-1}H_{L,k-1} + V_{k+1}H_{V,k+1} = L_k H_{L,k} + V_k H_{V,k}$$
(11)

2C + 3 eqns., 2C + 3 unks. Solved!

Where H_L and H_V are the specific enthalpies of the liquid and vapor streams (J/kgmole), respectively. These enthalpies are calculated by the simulator as functions of the temperature, pressure and composition using the specified thermodynamic package.

Notice that the solution of the tray equations requires the iterative solution of the flash equations, similar to those solved in the notes on Flash Distillation. Furthermore, because

the inlet streams to the tray are outlet streams from the tray above and the tray below, the complete solution of the column equations requires very sophisticated iteration algorithms. Process simulators possess these algorithms and are very useful for solving these equations.

Summary

These notes have dealt with the design of multicomponent distillation columns. The need for the definition of key components was introduced and the short cut design method was presented in detail. This included the estimation of the minimum reflux ratio at total reflux by the Fenske equation, the estimation of the minimum reflux ratio by the Underwood equation, and the estimation of the number of equilibrium stages at a specified reflux ratio by the Gilliland correlation.

A brief glance at the equations involved in the rigorous distillation models available in process simulators is also included.

Review Questions

 How many specifications are needed to define a column with C components in its feed stream and two product streams? How many of these are associated with the feed stream?

- List the five column specifications not associated with the feed stream required to design the column by the shortcut method.
- 3. Why is it necessary to select *key components* to design a multicomponent distillation column?
- 4. In order to solve the mass balances on a distillation column, what assumptions must be made on the lighter-thanlight-key (LLK) components and on the heavier-than-heavykey (HHK) components?
- 5. In the short-cut design method, for what is the Fenske equation used? For what is the Underwood equation used? For what is the Gilliland correlation used?
- 6. List the five column specifications that must be made to solve the rigorous distillation model. Why is this model called a *rating* model?

Problems

1. Design of a Multicomponent Distillation Column. The feed to a conventional distillation column is 30% vaporized at the conditions of the feed plate. Given below are the feed relative volatilities and the of composition the components. It is desired to have no more than 2 mole% of component C in the distillate, and no more than 1 mole% of component B in the bottoms product. Draw a schematic of the column showing all the problem data on the diagram and, using a reasonable reflux ratio, determine the number of actual stages required for an over-all efficiency of 60%, a total condenser and a partial reboiler. Report also the location of the feed stage, the flows and compositions of

the product streams, and the recoveries of the two key components. State all assumptions.

Component	Feed mole	fraction	α
A	0.06		2.1
В	0.43		1.7
С	0.47		1.0
D	0.04		0.65

2. Distillation of Mixture in Phenol Process. In a phenol process, a distillation column is to separate 914 kmole/hr of a liquid mixture, saturated at 1 atm, to recover 97.5% of the phenol in the bottoms product which is to contain no more than 0.001 mole fraction AMS (alpha-methyl styrene). The column is to operate at 1 psia at the top with a total pressure drop of 7.5 psi from bottom to top. Under these conditions, the K values given below apply. Draw a schematic of the column showing all problem data and, using a reasonable reflux ratio determine the number of actual trays for an over-all column efficiency of 65%, a total condenser and a partial reboiler. Report also the location of the feed stage, the flows and compositions of the product streams, and the recoveries of the two key components. State all assumptions.

Component	Feed mole fraction	n Kattop	K at bottom
Cumene	0.060	1.544	5.020
AMS	0.214	0.932	3.364
Phenol	0.695	0.793	1.008
MPK	0.031	0.275	0.228

3. Design of a Distillation Column to Separate Aromatics. A column is to separate 5,100 kmole/hr of a saturated liquid mixture at 20 psia to recover 99% of the ethylbenzene in

the bottoms product which is to contain no more than 0.6 mole% toluene. The column is to operate at atmospheric pressure at the top with a total pressure drop of 11 psi from bottom to top. Under these conditions, the K values given below apply. Draw a schematic of the column showing the problem data and, using a reasonable reflux ratio determine the number of actual trays for an over-all column efficiency of 65%, a total condenser and a partial reboiler. Report also the location of the feed stage, the flows and compositions of the product streams. State all assumptions.

Component	Feed mole	fraction	K at top	K at bottom
Benzene	0.05		1.875	3.571
Toluene	0.45		0.807	1.820
Ethylbenze	ne 0.40		0.388	1.006
p-Xylene	0.10		0.352	0.944

4. Separation of a Mixture of Xylenes. (based on McCabe, Smith, and Harriott, 7th edition, Problem 22.5, page 762) A saturated liquid mixture of xylenes plus other aromatics is separated in a large fractionating column operating at 18 psia. The following are the feed compositions and relative volatilities of the components:

	Feed mole fraction	n Relative Volatility
Ethyl-benzene	0.094	1.23
p-Xylene	0.151	1.15
m-Xylene	0.248	1.13
o-Xylene	0.472	1.0
n-Propyl-benzen	e 0.035	0.70

It is desired to recover 99% of the o-Xylene in the bottoms with no more than 0.5 mole% m-Xylene. Draw a schematic of the column showing the problem data and, using a reasonable reflux ratio determine the number of actual trays for an over-all column efficiency of 65%, a total condenser and a partial reboiler. Report also the location of the feed stage, the flows and compositions of the product streams. State all assumptions.

5. Column Design for Styrene Process. A distillation column in the Styrene process is to separate the benzene and toluene by-products from the unreacted ethylbenzene and styrene product. The feed compositions and equilibrium coefficients are as follows:

Component Feed	a mole fraction	K at top	K at bottom
Benzene	0.0576	1.568	4.157
Toluene	0.0529	0.664	2.111
Ethylbenzene	0.2869	0.3144	1.166
Styrene	0.6026	0.2292	0.918

It is desired to have a distillation product with no more than 0.1 mole% ethylbenzene and a bottoms product with no more than 0.1 mole% toluene. Determine the actual number of trays required for 50% over-all column efficiency at a reasonable reflux ratio. Report also the product rates and mole fractions, the liquid and vapor flows in the rectifying and stripping sections of the column, and the recoveries of the key components. The feed rate is 1,200

kmole/hr and it is saturated liquid at the conditions of the feed plate.

6. Column Design for VCM Process. A distillation column in the VCM process is to separate the HCl by-product from the unreacted ethylene di-chloride (EDC) and vinyl chloride (VCM) product. The feed rate is 1,600 kmole/hr and it enters 30% vapor on a molar basis. The feed compositions and equilibrium coefficients are as follows:

Component	Feed mole fraction	K at top	K at bottom
HCl	0.355	1.010	3.32
VCM	0.355	0.148	1.27
EDC	0.290	0.00632	0.40

It is desired recover 99.95% of the VCM and have a bottoms product with no more than 20 mole ppm (parts per million) HCl. Determine the actual number of trays required for 50% over-all column efficiency at a reasonable reflux ratio. Report also the product rates and mole fractions, the liquid and vapor flows in the rectifying and stripping sections of the column, and the recoveries of the key components.

7. Column Design for Phenol Process. A distillation column in the phenol process is to separate the acetone byproduct and unreacted cumene from the phenol product and MPK side product. It is desired to recover 99.9% of the phenol and remove 99.9% of the AMS. The feed is saturated liquid

entering at the rate of 2,700 kmole/hr and the compositions given below along with the equilibrium coefficients:

Component	Feed mole	fraction	K at top	K at bottom
Acetone	0.44		4.36	37.91
Cumene	0.05		0.135	3.38
Phenol	0.44		0.0574	0.903
MPK	0.07		0.0258	0.224

Determine the actual number of trays required for 50% overall column efficiency at a reasonable reflux ratio. Report also the product rates and mole fractions and the liquid and vapor flows in the rectifying and stripping sections of the column.

8. **AMS-Phenol Column Design.** A distillation column in the phenol process is to separate the AMS side product from the phenol product and the MPK. The feed is a saturated liquid and enters at 600 kmole/hr. The feed compositions and equilibrium coefficients are as follows:

Component	Feed	mole	fraction	K	at top	K	at	bottom
AMS		0.140)		1.001		3.	94
Phenol		0.810)		0.946		1.	020

The distillate product must contain no more than 1.5 mole% phenol and the bottoms product must contain no more than 100 mole ppm (parts per million) AMS. Determine the actual number of trays required for 50% over-all column efficiency at a reasonable reflux ratio. Report also the product rates and mole fractions, the liquid and vapor flows in the rectifying and stripping sections of the column, and the recoveries of the key components.