

SEPARATION PROCESSES

Example

12.1 Optimal Design and Operation of a Conventional Staged-Distillation Column	443
12.2 Optimization of Flow Rates in a Liquid–Liquid Extraction Column	448
12.3 Fitting Vapor–Liquid Equilibrium Data Via Nonlinear Regression	451
12.4 Determination of the Optimal Reflux Ratio for a Staged-Distillation Column	453
References	458
Supplementary References	458

SEPARATIONS ARE AN important phase in almost all chemical engineering processes. Separations are needed because the chemical species from a single source stream must be sent to multiple destinations with specified concentrations. The sources usually are raw material inputs and reactor effluents; the destinations are reactor inputs and product and waste streams. To achieve a desired species allocation you must determine the best types and sequence of separators to be used, evaluate the physical or chemical property differences to be exploited at each separator, fix the phases at each separator, and prescribe operating conditions for the entire process. Optimization is involved both in the design of the equipment and in the determination of the optimal operating conditions for the equipment.

A wide variety of separation processes exist (Meloan, 1999), including

Centrifugation	Flotation
Chromatography	Freeze drying
Dialysis	Ion exchange
Distillation	Membranes
Electrophoresis	Osmosis
Extraction	Zone melting
Filtration	

Although each type of process is based on different physical principles, the mathematical models used to represent a process are surprisingly similar. Usually the equations are material or energy balances, either steady-state (most often) or dynamic, corresponding to fundamental laws, and empirical equilibrium relations. The equations may involve discrete or continuous variables depending on the simplifying assumptions made. For example, for a staged-distillation column the typical assumptions might include one or more of the following:

1. The hold-up liquid on each plate is completely mixed.
2. A constant hold-up exists on each plate, in the reboiler, and in the condenser-accumulator system.
3. The fluid dynamic response time is negligible.
4. The effects of pressure changes in various sections of the column on the physical properties of the system being distilled are negligible.
5. The saturated liquid and vapor enthalpies can be expressed as a linear function of compositions.
6. All fluid streams are single phase, and liquid entrainment and vapor hold up are negligible.
7. The column operates adiabatically; heat lost to the atmosphere is negligible.
8. The liquid and vapor compositions leaving a plate are a function only of the compositions in the column and experimental plate efficiencies, and can be described as a linear function of corrected compositions at various sections of the column.
9. At a constant operating steam pressure, the heat transfer in the reboiler is a function of composition.

Many of these assumptions are made to reduce the complexity of the mathematical model for the distillation process. Some may have negligible adverse effects in a specific process, whereas others could prove to be too restrictive.

This chapter contains examples of optimization techniques applied to the design and operation of two of the most common staged and continuous processes, namely, distillation and extraction. We also illustrate the use of parameter estimation for fitting a function to thermodynamic data.

EXAMPLE 12.1 OPTIMAL DESIGN AND OPERATION OF A CONVENTIONAL STAGED-DISTILLATION COLUMN

Distillation is probably the most widely used separation process in industry. Various classes of optimization problems for steady-state distillation are, in increasing order of complexity,

1. Determine the optimal operating conditions for an existing column to achieve specific performance at minimum cost (or minimum energy usage) given the feed(s). Usually, the manipulated (independent) variables are indirect heat inputs, cooling stream inputs, and product flow rates. The number of degrees of freedom is most likely equal to the number of product streams. Specific performance is measured by specified component concentrations or fractional recoveries from the feed (specifications leading to equality constraints) or minimum (or maximum) concentrations and recoveries (specifications leading to inequality constraints). In principle, any of the specified quantities as well as costs can be calculated from the values of the manipulated variables given the mathematical model (or computer code) for the column. When posed as described earlier, the optimization problem is a nonlinear programming problem often with implicit nested loops for calculation of physical properties. If the number of degrees of freedom is reduced to zero by specifications placed on the controlled variables, the optimization problem reduces to the classic problem of distillation design that requires just the solution of a set of nonlinear equations.
2. A more complex problem is to determine not only the values of the operating conditions as outlined in item 1 but also the (minimum) number of stages required for the separation. Because the stages are discrete (although in certain examples in this book we have treated them as continuous variables), the problem outlined in item 1 becomes a nonlinear mixed-integer programming problem (see Chapter 9). In this form of the design problem, the costs include both capital costs and operating costs. Capital costs increase with the number of stages and internal column flow rates, whereas operating costs decrease up to a certain point.
3. An even more difficult problem is to determine the number of stages and the optimal locations for the feed(s) and side stream(s) withdrawal. Fortunately, the range of candidates for stage locations for feed and withdrawals is usually small, and from a practical viewpoint the objective function is usually not particularly sensitive to a specific location within the appropriate range.

Optimization of distillation columns using mathematical programming, as opposed to other methods, has been carried out using many techniques, including search methods such as Hooke and Jeeves (Srygley and Holland, 1965), mixed-integer nonlinear programming (MINLP) (Frey et al., 1997; and Bauer and Stichlmair, 1998), genetic algorithms (Fraga and Matias, 1996), and successive quadratic programming (SQP) (Schmid and Biegler, 1994), which is the technique we use in this example. The review by Skogestad (1997) treats many of the various issues involved in the optimization of distillation columns beyond those we illustrate here.

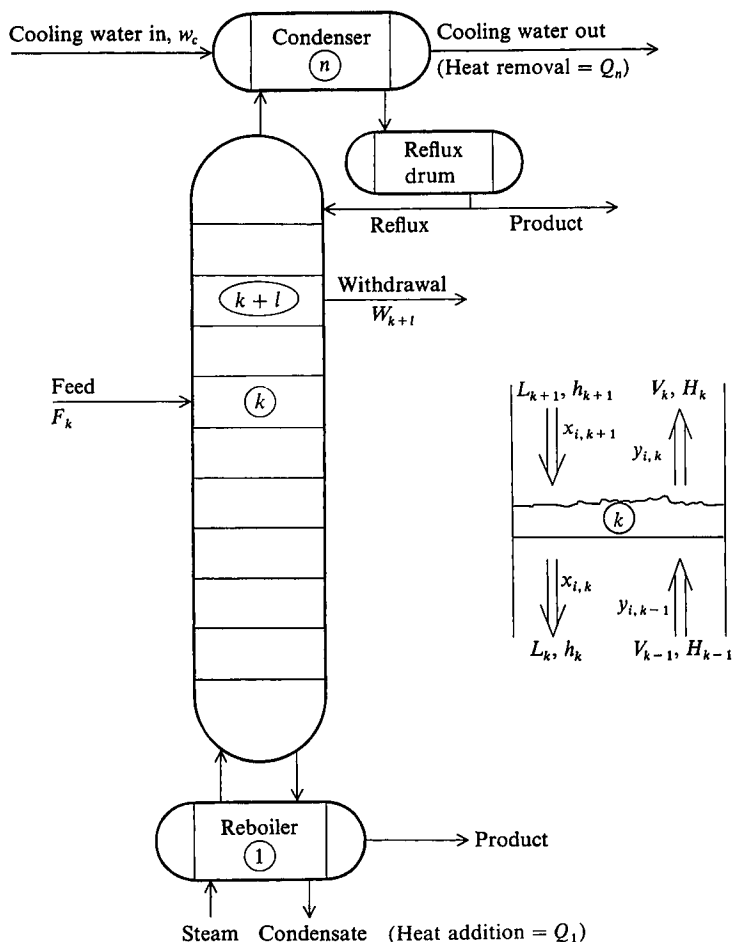


FIGURE E12.1
Schematic of a staged distillation column.

This example focuses on the design and optimization of a steady-state staged column. Figure E12.1 shows a typical column and some of the notation we will use, and Table E12.1A lists the other variables and parameters. Feed is denoted by superscript F . Withdrawals take the subscripts of the withdrawal stage. Superscripts V for vapor and L for liquid are used as needed to distinguish between phases. If we number the stages from the bottom of the column (the reboiler) upward with $k = 1$, then $V_0 = L_1 = 0$, and at the top of the column, or the condenser, $V_n = L_{n+1} = 0$. We first formulate the equality constraints, then the inequality constraints, and lastly the objective function.

The equality constraints. The process model comprises the equality constraints. For a conventional distillation column we have the following typical relations:

TABLE E12.1A
Notation for distillation example

F_k	flow of feed into stage k , moles
h_k	liquid enthalpy (a function of p_k , T_k , and \mathbf{x}_k) on stage k
H_k	vapor enthalpy (a function of p_k , T_k , and \mathbf{y}_k) on stage k
k	stage index number, $k = 1, \dots, n$
$K_{i,k}$	equilibrium constant for component i for the mixture on stage k (a function of p_k , T_k , \mathbf{x}_k , \mathbf{y}_k)
L_k	flow of liquid from stage k , moles
m	number of components, $i = 1, \dots, m$
p_k	pressure on stage k
Q_k	heat transfer flow to stage k (positive when into stage)
T_k	temperature on stage k
V_k	flow of vapor from stage k , moles
W_k	withdrawal stream from stage k , moles
$x_{i,k}$	mole fraction of component i on stage k in the liquid phase
$y_{i,k}$	mole fraction of component i on stage k in the vapor phase

1. Total material balances (one for each stage k)

$$F_k^L + F_k^V + V_{k-1} + L_{k+1} = V_k + L_k + W_k^V + W_k^L \quad (a)$$

(F_k and W_k are ordinarily not involved in most of the stages)

2. Component material balances (one for each component i for each stage k)

$$x_{i,k}^F F_k^L + y_{i,k}^F F_k^V + y_{i,k-1} V_{k-1} + x_{i,k+1} L_{k+1} = y_{i,k} V_k + x_{i,k} L_k + y_{i,k} W_k^V + x_{i,k} W_k^L \quad (b)$$

3. Energy balance (one for each stage)

$$Q_k + h_k^F F_k + H_{k-1} V_{k-1} + h_{k+1} L_{k+1} = H_k V_k + h_k L_k + H_k W_k^V + h_k W_k^L \quad (c)$$

4. Equilibrium relations for liquid and vapor at each stage (one for each stage)

$$y_{i,k} = K_{i,k} x_{i,k} \quad (d)$$

5. Relation between equilibrium constant and p , T , x , y (one for each stage)

$$K_{i,k} = K_i(p_k, T_k, \mathbf{x}_k, \mathbf{y}_k) \quad (e)$$

6. Relation between enthalpies and p , T , x , y (one for each stage)

$$h_k = h(p_k, T_k, \mathbf{x}_k) \quad (f)$$

$$H_k = H(p_k, T_k, \mathbf{y}_k) \quad (g)$$

The preceding classic set of algebraic equations form a well-defined sparse structure that has been analyzed extensively. Innumerable techniques of solution have been proposed for problems with 0 degrees of freedom, that is, the column operating or design variables are completely specified.

Our interest here in posing an optimization problem is to have one or more degrees of freedom left after prespecifying the values of most of the independent variables. Frequently, values are given for the following parameters:

- (a) Number of stages
- (b) Flow rate, composition, and enthalpy of the feed(s)
- (c) Location of the feed(s) and side stream withdrawal(s)
- (d) Flow rate of the side stream(s)
- (e) Heat input rate to each stage except one
- (f) Stage pressures (based on column detailed design specifications)

Reactive distillation involves additional degrees of freedom (Mujtaba and Macchietto, 1997). If the controllable parameters remaining to be specified, namely (1) one heat input, and (2) the flow rate of the product (or the reflux ratio), are determined via optimization, all of the values of V_k , L_k , T_k , $x_{i,k}$, and $y_{i,k}$ and the enthalpies can be calculated. More than 2 degrees of freedom can be introduced by eliminating some of the prespecified parameters values.

7. Certain implicit equality constraints exist

Because of the way the model is specified, you must take into account the following additional equations as constraints in the column model:

$$\sum_{i=1}^m x_{i,k} = 1 \quad (h)$$

$$\sum_{i=1}^m y_{i,k} = 1 \quad (i)$$

The inequality constraints. Various kinds of inequality constraints exist, such as requiring that all of the $x_{i,k}$, $y_{i,k}$, Q_k , F_k , W_k , and so on be positive, that upper and lower bounds be imposed on some of the product stream concentrations, and specification of the minimum recovery factors. A recovery factor for stage k is the ratio

$$\frac{x_{i,k}W_k^L + y_{i,k}W_k^V}{\sum_i (x_{i,k}F_k^L + y_{i,k}F_k^V)}$$

The objective function. The main costs of operation are the heating and cooling costs that are related to Q_1 and Q_n , respectively. We assume all the other values of Q_k are zero. Q_n is determined from the energy balance, so that Q_1 is the independent variable. The cost of operation per annum is assumed to be directly proportional to Q_1 because the maintenance and cooling costs are relatively small and the capital costs per annum are already fixed. Consequently, the objective function is relatively simple:

$$\text{Minimize: } Q_1 \quad (j)$$

As posed here, the problem is a nonlinear programming one and involves nested loops of calculations, the outer loop of which is Equation (j) subject to Equations (a) through (i), and subject to the inequality constraints. If capital costs are to be included in the objective function, refer to Frey and colleagues (1997).

Results for a specific problem with 5 degrees of freedom. For illustration, we use the data of Sargent and Gaminibandara (1976) for the objective function (j).

The problem is to determine the location and individual amounts of the feeds given the following information.

A column of four stages exists analogous to that shown in Figure E12.1 except that more than one feed can exist (the reboiler is stage 1 and the condenser is stage 4). Feed and product specifications are

$$\text{Total feed} = 100 \text{ lb mol/h liquid}$$

$$h_F = 4000 \text{ Btu/lb mol}$$

$$x_1 = 0.05 \text{ (C}_3\text{H}_8\text{)}$$

$$x_2 = 0.15 \text{ (i-C}_4\text{H}_{10}\text{)}$$

$$x_3 = 0.25 \text{ (n-C}_4\text{H}_{10}\text{)}$$

$$x_4 = 0.20 \text{ (i-C}_5\text{H}_{12}\text{)}$$

$$x_5 = 0.35 \text{ (n-C}_5\text{H}_{12}\text{)}$$

$$\text{Top product} = 10 \text{ lb mol/h liquid}$$

$$x_5 \leq 0.07$$

The equality constraints are Equations (a)–(i) plus

$$\sum_{k=1}^4 F_k = 100 \quad (k)$$

The inequality constraints are ($k = 1, \dots, 4$)

$$Q_1 \geq 0 \quad (l)$$

$$Q_4 \leq 0 \quad (m)$$

$$x_{i,k} \geq 0 \quad (n)$$

$$y_{i,k} \geq 0 \quad (o)$$

$$F_k \geq 0 \quad (p)$$

$$x_{5,4} \leq 0.07 \quad (q)$$

This problem has 5 degrees of freedom, representing the five variables Q_1 , F_1 , F_2 , F_3 , and F_4 .

Various rules of thumb and empirical correlations exist to assist in making initial guesses for the values of the independent variables. All the values of the feeds here can be assumed to be equal initially. If the reflux ratio is selected as an independent variable, a value of 1 to 1.5 times the minimum reflux ratio is generally appropriate.

To solve the problem a sequential quadratic programming code was used in the outer loop of calculations. Inner loops were used to evaluate the physical properties. Forward-finite differences with a step size of $h = 10^{-7}$ were used as substitute for the derivatives. Equilibrium data were taken from Holland (1963). The results shown in Table E12.1B were essentially the same as those obtained by Sargent and Gaminibandara.

TABLE E12.1B
Results of optimization

Variable	Initial guess for the variable	Optimal values for the variable
F_1	25	23.7
F_2	25	0
F_3	25	0
F_4	25	76.3
Q_1	5.0×10^6	3.38×10^5
$x_{5,4}$	—	0.07

We can conclude that it is possible to use some of the cold feed as reflux in the top stage without voiding the product composition specification. This outcome is not an obvious choice for the problem specifications.

EXAMPLE 12.2 OPTIMIZATION OF FLOW RATES IN A LIQUID-LIQUID EXTRACTION COLUMN

Liquid-liquid extraction is carried out either (1) in a series of well-mixed vessels or stages (well-mixed tanks or in plate column), or (2) in a continuous process, such as a spray column, packed column, or rotating disk column. If the process model is to be represented with integer variables, as in a staged process, MILNP (Glanz and Stichlmair, 1997) or one of the methods described in Chapters 9 and 10 can be employed. This example focuses on optimization in which the model is composed of two first-order, steady-state differential equations (a plug flow model). A similar treatment can be applied to an axial dispersion model.

Figure E12.2a illustrates a typical steady-state continuous column. The model and the objective function are formulated as follows.

The process model. Under certain conditions, the plug flow model for an extraction process has an analytical solution. Under other conditions, numerical solutions of the equations must be used. As a practical matter, specifying the model so that an analytical solution exists means assuming that the concentrations are expressed on a solute-free mole basis, that the equilibrium relation between Y and X is a straight line $Y^* = mX + B$ (i.e., not necessarily through the origin), and that the operating line is straight, that is, the phases are insoluble. Then the model is

$$\frac{dX}{dZ} - N_{OX}(X - Y) = 0 \quad (a)$$

$$\frac{dY}{dZ} - FN_{OX}(X - Y) = 0 \quad (b)$$

where F = extraction factor (mv_X/v_Y)

m = distribution coefficient

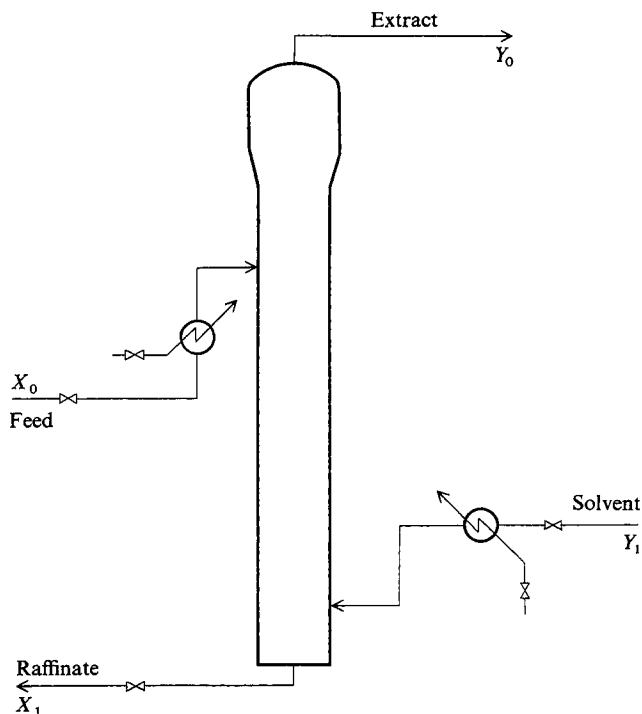
N_{OX} = number of transfer units

v_X, v_Y = superficial velocity in raffinate, extract phase, respectively

X = dimensionless raffinate phase concentration

Y = dimensionless extract phase concentration

Z = dimensionless contactor length

**FIGURE E12.2a**

Extraction column schematic for Example 12.2. (The internal rotating disks are not shown.)

Figure E12.2a shows the boundary conditions X_0 and Y_1 . Given values for m , N_{OX} , and the length of the column, a solution for Y_0 in terms of v_X and v_Y can be obtained; X_1 is related to Y_0 and F via a material balance: $X_1 = 1 - (Y_0/F)$. Hartland and Mecklenburgh (1975) list the solutions for the plug flow model (and also the axial dispersion model) for a linear equilibrium relationship, in terms of F :

$$Y_0 = \frac{F\{1 - \exp[N_{OX}(1 - F)]\}}{1 - F \exp[N_{OX}(1 - F)]} \quad (c)$$

In practice, N_{OX} is calculated from experimental data by least squares or from an explicit relation for the plug flow model.

$$N_{OX} = \left(\frac{1 - X_1}{X_1 + Y_0 - 1} \right) \ln \left(\frac{X_1}{1 - Y_0} \right) \quad (d)$$

Jackson and Agnew (1980) summarized a number of correlations for N_{OX} such as

$$N_{OX} = 4.81 \left(\frac{v_X}{v_Y} \right)^{0.24} \quad (e)$$

The value of $m = 1.5$.

Inequality constraints. Implicit constraints exist because of the use of dimensionless variables

$$X_0 \leq X \leq X_1$$

$$Y_1 \leq Y \leq Y_0 \quad (f)$$

Constraints on v_x and v_y are upper and lower bounds such as

$$0.05 < v_x < 0.25$$

$$0.05 < v_y < 0.30 \quad (g)$$

and the flooding constraint

$$v_x + v_y \leq 0.20 \quad (h)$$

Objective function. The objective function is to maximize the total extraction rate for constant disk rotation speed subject to the inequality and equality constraints:

$$\text{Maximize: } f = v_y Y_0 \quad (i)$$

Results of the optimization. Figure E12.2b illustrates contours of the objective function for the plug flow model; the objective function (i) was optimized by the GRG

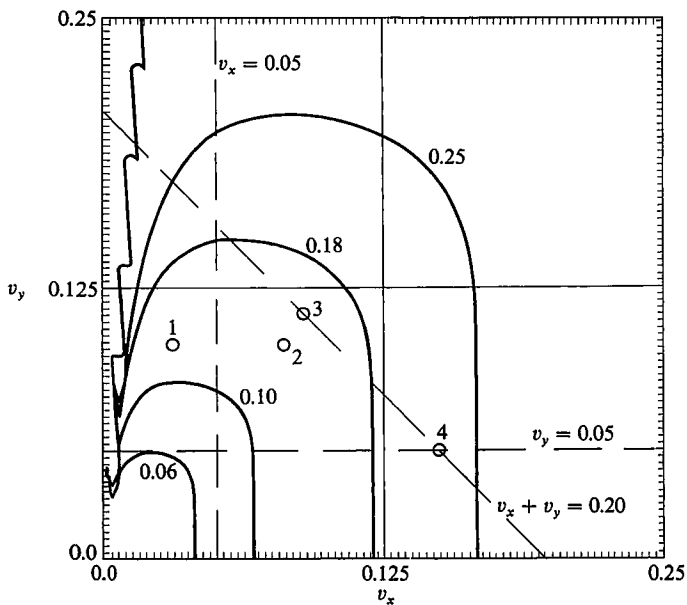


FIGURE E12.2b

Contours (the heavy lines) for the objective function of extraction process. Points 1, 2, 3, and 4 indicate the progress of the reduced-gradient method toward the optimum (point 4).

(generalized reduced-gradient) method. For small values of v_x (< 0.01), the contours drop off quite rapidly. The starting point (point 1)

$$v_x = 0.03$$

$$v_y = 0.10$$

is infeasible. Points 2, 3, and 4 in Figure E12.2b show the change as the vector of independent variables moves toward the optimum. Point 2 indicates the first feasible values of v_x and v_y (0.08, 0.10), point 3 indicates where the flooding constraint (h) is active, and point 4 is the constrained optimum (0.15, 0.05). The value of the objective function at point 4 is 0.225.

EXAMPLE 12.3 FITTING VAPOR-LIQUID EQUILIBRIUM DATA VIA NONLINEAR REGRESSION

Valid physical property relationships form an important feature of a process model. To validate a model, representative data must fit by some type of correlation using an optimization technique. Nonlinear regression instead of linear regression may be involved in the fitting. We illustrate the procedure in this example.

Separation systems include in their mathematical models various vapor-liquid equilibrium (VLE) correlations that are specific to the binary or multicomponent system of interest. Such correlations are usually obtained by fitting VLE data by least squares. The nature of the data can depend on the level of sophistication of the experimental work. In some cases it is only feasible to measure the total pressure of a system as a function of the liquid phase mole fraction (no vapor phase mole fraction data are available).

Vapor-liquid equilibria data are often correlated using two adjustable parameters per binary mixture. In many cases, multicomponent vapor-liquid equilibria can be predicted using only binary parameters. For low pressures, the equilibrium constraint is

$$x_i \gamma_i p_i^{\text{sat}} = y_i p \quad (i = 1, 2) \quad (a)$$

where p = the total pressure

p_i^{sat} = the saturation pressure of component i

x_i = the liquid phase mole fraction of component i

γ_i = the activity coefficient

y_i = the vapor phase mole fraction

The van Laar model for a binary mixture is

$$\ln \gamma_1 = A_{12} \left[\frac{A_{21} x_2}{A_{12} x_1 + A_{21} x_2} \right]^2 \quad (b)$$

and

$$\ln \gamma_2 = A_{21} \left[\frac{A_{12} x_1}{A_{12} x_1 + A_{21} x_2} \right]^2 \quad (c)$$

where A_{12} and A_{21} are binary constants that are adjusted by optimization to fit the calculated data for x_i . To use total pressure measurements we write

$$p = y_1 p + y_2 p \quad (d)$$

TABLE E12.3
Experimental VLE data for the system
(1) Water. (2) 1,4 dioxane at 20°C.

Experimental data		Predicted values		
x_1	$p^{\text{expt}}(\text{mmHg})$	p^{calc}	p	y^{calc}
0.00	28.10	28.10	0.00	0.0
0.10	34.40	34.20	-0.20	0.2508
0.20	36.70	36.95	0.25	0.3245
0.30	36.90	36.97	0.07	0.3493
0.40	36.80	36.75	-0.05	0.3576
0.50	36.70	36.64	-0.06	0.3625
0.60	36.50	36.56	0.06	0.3725
0.70	35.40	35.36	-0.04	0.3965
0.80	32.90	32.84	-0.06	0.4503
0.90	27.70	27.72	0.02	0.5781
1.00	17.50	17.50	0.00	1.0

Antoine constants:

$\log p^{\text{sat}} = a_1 - \frac{a_2}{T + a_3}$

p^{sat} : mmHg
 T : °C

	a_1	a_2	a_3	Range
(1) Water	8.07131	1730.630	233.426	(1–100°C)
(2) 1,4 dioxane	7.43155	1554.679	240.337	(20–105°C)

Note: Data reported by Hororka et al. (1936).

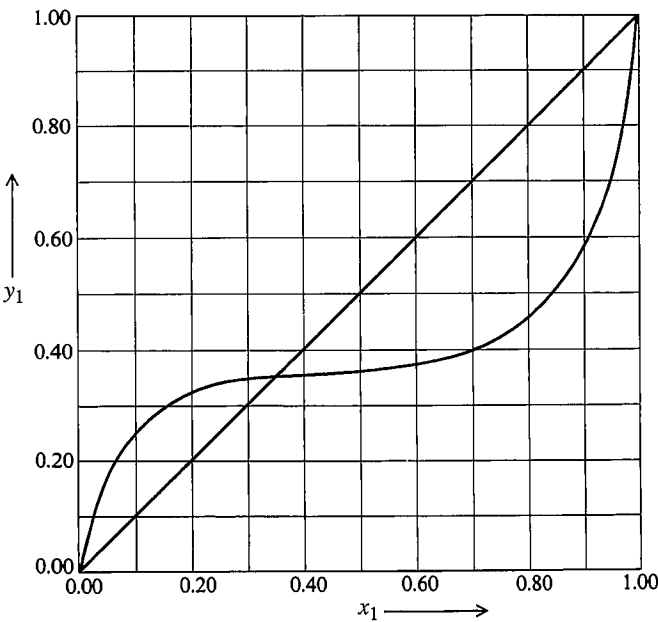


FIGURE E12.3
Experimental vapor–liquid equilibrium data, Example 12.3.
[Source: Gmehling et al. (1981).]

or, using Equations (a)–(c)

$$p = x_1 \exp \left[A_{12} \left(\frac{A_{21}x_2}{A_{12}x_1 + A_{21}x_2} \right)^2 \right] p_i^{\text{sat}} + x_2 \exp \left[A_{21} \left(\frac{A_{12}x_1}{A_{12}x_1 + A_{21}x_2} \right)^2 \right] p_2^{\text{sat}} \quad (e)$$

The saturation pressures can be predicted at a given temperature using the Antoine equation. For a given temperature and a binary system ($x_2 = 1 - x_1$)

$$p = p(x_1, A_{12}, A_{21}) \quad (f)$$

so that the two binary coefficients may be determined from experimental values of p versus x_1 by nonlinear least squares estimation (regression), that is, by minimizing the objective function

$$f = \sum_{i=1}^n (p_j^{\text{calc}} - p_j^{\text{expt}})^2 \quad (g)$$

where n is the number of data points.

In the book, *Vapor-Liquid Equilibrium Data Collection*, Gmehling and colleagues (1981), nonlinear regression has been applied to develop several different vapor-liquid equilibria relations suitable for correlating numerous data systems. As an example, p versus x_1 data for the system water (1) and 1,4 dioxane (2) at 20.00°C are listed in Table E12.3. The Antoine equation coefficients for each component are also shown in Table E12.3. A_{12} and A_{21} were calculated by Gmehling and colleagues using the Nelder-Mead simplex method (see Section 6.1.4) to be 2.0656 and 1.6993, respectively. The vapor phase mole fractions, total pressure, and the deviation between predicted and experimental values of the total p

$$\Delta p_j = p_j^{\text{calc}} - p_j^{\text{expt}}$$

are listed in Table E12.3 for increments of $x_1 = 0.10$. The mean Δp is 0.09 mmHg for pressures ranging from 17.5 to 28.10 mmHg. Figure E12.3 shows the predicted y_1 versus x_1 data; note that the model predicts an azeotrope at $x_1 = y_1 = 0.35$.

EXAMPLE 12.4 DETERMINATION OF THE OPTIMAL REFLUX RATIO FOR A STAGED-DISTILLATION COLUMN

Once a distillation column is in operation, the number of trays is fixed and very few degrees of freedom can be manipulated to minimize operating costs. The reflux ratio frequently is used to control the steady-state operating point. Figure E12.4a shows typical variable cost patterns as a function of the reflux ratio. The optimization of reflux ratio is particularly attractive for columns that operate with

1. High reflux ratio
2. High differential product values (between overhead and bottoms)
3. High utility costs
4. Low relative volatility
5. Feed light key far from 50 percent

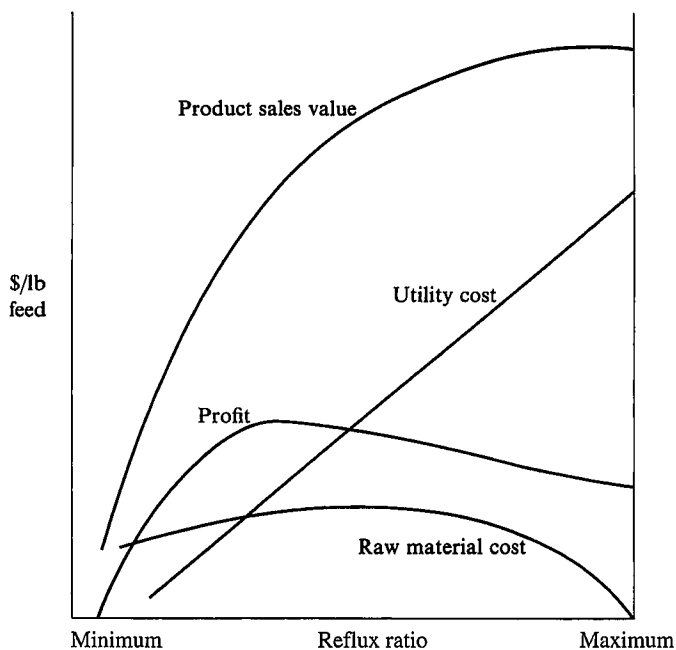


FIGURE E12.4a
Variable cost trade-offs for a distillation column.

In this example we illustrate the application of a one-dimensional search technique from Chapter 5 to a problem posed by Martin and coworkers (1981) of obtaining the optimal reflux ratio in a distillation column.

Martin and coworkers described an application of optimization to an existing tower separating propane and propylene. The lighter component (propylene) is more valuable than propane. For example, propylene and propane in the overhead product were both valued at \$0.20/lb (a small amount of propane was allowable in the overhead), but propane in the bottoms was worth \$0.12/lb and propylene \$0.09/lb. The overhead stream had to be at least 95 percent propylene. Based on the data in Table E12.4A, we will determine the optimum reflux ratio for this column using derivations provided by McAvoy (personal communication, 1985). He employed correlations for column performance (operating equations) developed by Eduljee (1975).

Equality constraints. The Eduljee correlation involves two parameters: R_m , the minimum reflux ratio, and N_m , the equivalent number of stages to accomplish the separation at total reflux. His operating equations relate N , α , X_F , X_D , and X_B (see Table E12.4A for notation) all of which have known values except X_B as listed in Table E12.4A. Once R is specified, you can find X_B by sequential solution of the three following equations.

TABLE E12.4A
Notation and values for the propane–propylene splitter

Symbol	Description	Value
B	Bottoms flow rate	
C_1	Reboiler heat cost	\$3.00/10 ⁶ Btu
C_2	Condenser cooling cost	\$0.00/10 ⁶ Btu
C_B	Value of propylene in bottoms	
C'_B	Value of propane in bottoms	
C_F	Cost per pound of propylene	
C'_F	Cost per pound of propane	
C_D	Value of propylene in overhead	
C'_D	Value of propane in overhead	
D	Distillate flow rate	
F	Feed rate	1,200,000 lb/day
L	Liquid flow rate	function of R (mol/day)
N	Number of equilibrium stages	94
N_m	Minimum equilibrium stages	function of reflux ratio, R
Q_C	Condenser load requirement	$Q_C \approx \lambda V$
Q_R	Reboiler heat requirement	$Q_R \approx \lambda V$
R	Reflux ratio	(To be optimized)
R_m	Minimum reflux ratio	11.17
U	Heavy key differential value	−\$0.08/lb
V	Vapor flow rate	function of R (mol/day)
W	Light key differential value	\$0.11/lb
X_B	Bottom light key mole fraction	(To be optimized)
X_D	Overhead light key mole fraction	0.95
X_F	Feed light key mole fraction	0.70
α	Relative volatility	1.105
λ	Latent heat	130 Btu/lb (avg. mixture)

First, calculate R_m

$$R_m = \frac{1}{(\alpha - 1)} \left[\frac{X_D}{X_F} - \alpha \frac{(1 - X_D)}{(1 - X_F)} \right] \quad (a)$$

Substitute the value of R_m in Equation (b) to find N_m

$$\left(\frac{N - N_m}{N + 1} \right) = 0.75 \left[1 - \left(\frac{R - R_m}{R + 1} \right)^{0.5668} \right] \quad (b)$$

Lastly, compute X_B from

$$N_m = \frac{\ln \{ [X_D / (1 - X_D)] \cdot [(1 - X_B) / X_B] \}}{\ln \alpha} \quad (c)$$

Equations (a)–(c) comprise equality constraints relating X_B and R .

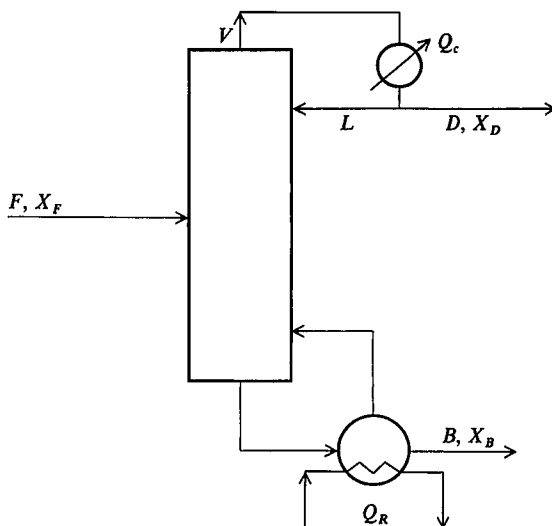


FIGURE E12.4b
Distillation column flow chart.

Once X_B is calculated, the overall material balance for the column shown in Figure E12.4b can be computed. The pertinent equations are (the units are moles)

$$F = D + B \quad (d)$$

$$X_F F = X_D D + X_B B \quad (e)$$

Equations (d) and (e) contain two unknowns: D and B , which can be determined once F , X_F , X_B , and X_D are specified. In addition, if the assumption of constant molal overflow is made, then the liquid L and vapor flows V are

$$L = RD \quad (f)$$

$$V = (R + 1)D \quad (g)$$

Objective function. Next we develop expressions for the income and operating costs. The operating profit f is given by

$$f = \text{Propylene sales} + \text{Propane sales} - \text{Utility costs} - \text{Raw material costs} \quad (h)$$

$$f = (C_D X_D D + C_B X_B B) + [C'_D(1 - X_D)D + C'_B(1 - X_B)B] \\ - [C_1 Q_R + C_2 Q_C] - [C_F X_F F + C'_F(1 - X_F)F] \quad (i)$$

The brackets [] indicate the correspondence between the words in Equation (h) and the symbols in Equation (i). Q_R is the reboiler heat requirement and Q_C is the cooling load.

Equation (i) can be rearranged by substituting for DX_D in the propylene sales and for BX_B in the propane sales using Equation (e) and defining $-W = C_B - C_D$ and $-U = C'_D - C'_B$ as follows

TABLE E12.4B
Iterations in quadratic interpolation test problem

Iteration	Left bracket		Center point		Right bracket		Interpolated values	
	<i>x</i>	<i>f</i>	<i>x</i>	<i>f</i>	<i>x</i>	<i>f</i>	<i>x</i>	<i>f</i>
1	16.00	3967.13	18.00	3922.14	20.00	4256.45	17.24	3872.22
2	18.00	3922.14	17.24	3872.22	16.00	3967.13	17.16	3870.79
3	17.24	3872.22	17.16	3870.79	16.00	3967.13	17.09	3870.21
4	17.16	3870.79	17.09	3870.21	16.00	3967.13	17.06	3870.18
5	17.09	3870.21	17.06	3870.18	16.00	3967.13	17.06	3870.17
Final solution								
<i>x</i> = 17.06								
<i>f</i> = 3870.17								

TABLE E12.4C
Sensitivity study at the reflux ratio optimum

Reflux ratio (<i>R</i>)	<i>X_B</i> (mol fraction)	Costs (\$/day)
17.07	0.0432	3870
18.77*	0.0303	4024
15.36*	0.0683	4159

*Indicates $1 / .07 \pm 10\%$

$$f = C_D X_F F + C'_B (1 - X_F) F - C_F X_F F - C'_F (1 - X_F) F - C_1 Q_R - C_2 Q_C - W X_B B - U (1 - X_D) D \quad (j)$$

Note that the first four terms of f are fixed values, hence these terms can be deleted from the expression for f in the optimization. In addition, it is reasonable to assume $Q_R \approx Q_C \approx \lambda V$. Lastly, the right-hand side of Equation (j) can be multiplied by -1 to give the final form of the objective function (to be minimized):

$$f_1 = (C_1 + C_2) \lambda V + W X_B B + U (1 - X_D) D \quad (k)$$

Note: λ must be converted to Btu/mol, and the costs to \$/mol.

Solution. Based on the data in Table E12.4A we minimized f_1 with respect to R using a quadratic interpolation one-dimensional search (see Chapter 5). The value of R_m from Equation (a) was 11.338. The initial bracket was $12 \leq R \leq 20$, and $R = 16, 18$, and 20 were selected for the initial three points. The convergence tolerance on the optimum required that f_1 should not change by more than 0.01 from one iteration to the next.

The iterative program incorporating the quadratic interpolation search yielded the results in Table E12.4B. The optimum reflux ratio was 17.06 and the cost, f_1 , was \$3870/day. Table E12.4C shows the variation in f_1 for ± 10 percent change in R . The profit function changes \$100/day or more.

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13

FLUID FLOW SYSTEMS

Example

13.1 Optimal Pipe Diameter	461
13.2 Minimum Work of Compression	464
13.3 Economic Operation of a Fixed-Bed Filter	466
13.4 Optimal Design of a Gas Transmission Network	469
References	478
Supplementary References	478