6

Specification of Design Variables

In the design of processes for physical separation of components by mechanisms involving mass and heat transfer, the first step usually consists of specification of process conditions or independent variables.

Mooson Kwauk, 1956

The solution to a multicomponent, multiphase, multistage separation problem is found in the simultaneous or iterative solution of, literally, hundreds of equations. This implies that a sufficient number of design variables is specified so that the number of unknown (output) variables exactly equals the number of (independent) equations. When this is done, a separation process is uniquely specified. If an incorrect number of design variables is chosen, multiple or inconsistent solutions or no solution at all will be found.

The computational difficulties attending the solution of large sets of frequently nonlinear equations are such that a judicious choice of design variables frequently ameliorates computational obstacles. In practice, however, the designer is not free to choose the design variables on the basis of computational convenience. More commonly he is confronted with a situation where the feed composition, the number of stages, and/or the product specifications are fixed and he must suitably arrange the equations so they can be solved.

An intuitively simple, but operationally complex, method of finding N_D, the number of *independent design variables*, *degrees of freedom*, or *variance* in the process, is to enumerate all pertinent variables N_V and to subtract from these the total number of independent equations N_E relating the variables.

$$N_D = N_V - N_E \tag{6-1}$$

This approach to separation process design was developed by Kwauk,[1] and a modification of his methodology forms the basis for this chapter.

Typically, the variables in a separation process can be *intensive variables* such as composition, temperature, or pressure; *extensive variables* such as flow rate or heat transferred; or equipment parameters such as the number of equilibrium stages. Physical properties such as enthalpy or K-values are not counted. The variables are relatively easy to enumerate; but to achieve an unambiguous count of N_E it is necessary to carefully seek out all independent relationships due to material and energy conservations, phase equilibrium restrictions, process specifications, and equipment configurations.

Separation equipment consists of physically identifiable elements (equilibrium stages, condensers, reboilers, etc.) as well as stream dividers and stream mixers. It is helpful to examine each element separately, prior to synthesizing the complete system.

6.1 Stream Variables

For each single-phase stream containing C components, a complete specification of intensive variables consists of $C-1$ mole fractions (or other concentration variables) plus temperature and pressure. This follows from the phase rule, which states that, for a single-phase system, the intensive variables are specified by $C-\mathcal{P}+2=C+1$ variables. To this number can be added the total flow rate, an extensive variable. Finally, although the missing mole fractions are often treated implicitly, it is preferable for completeness to include these missing mole fractions in the list of stream variables and then to include in the list of equations the mole fraction constraint

$$\sum_{i=1}^{C} \text{mole fractions} = 1.0$$

Thus, associated with each stream are $C+3$ variables. For example, for a liquid-phase stream, the variables might be

Liquid mole fractions $x_1, x_2, \ldots, x_C$.

Total molal flow rate L.

Temperature T.

Pressure P.

6.2 Adiabatic Equilibrium Stage

For a single adiabatic equilibrium stage with two entering streams and two exit streams, as shown in Fig. 6.1, the only variables are those associated with the streams. Thus

$$N_V = 4(C+3) = 4C+12$$

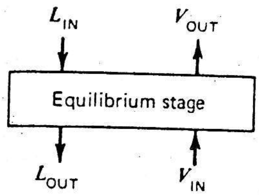


Figure 6.1. Adiabatic equilibrium stage.

The exit streams V_{OUT} and L_{OUT} are in equilibrium so there are equilibrium restrictions as well as component material balances, a total material balance, an enthalpy balance, and mole fraction constraints. Thus N_E, the number of equations relating these variables, is

Equations	Number of Equations
Pressure equality, $P_{V_{OUT}} = P_{L_{OUT}}$	1
Temperature equality, $T_{V_{OUT}} = T_{L_{OUT}}$	1
Phase equilibrium relationships, $(y_i)_{V_{OUT}} = K_i(x_i)_{L_{OUT}}$	C
Component material balances, $L_{IN}(x_i)_{L_{IN}} + V_{IN}(y_i)_{V_{IN}} = L_{OUT}(x_i)_{L_{OUT}} + V_{OUT}(y_i)_{V_{OUT}}$	$C-1$
Total material balance, $L_{IN} + V_{IN} = L_{OUT} + V_{OUT}$	1
Adiabatic enthalpy balance, $H_{L_{IN}}L_{IN} + H_{V_{IN}}V_{IN} = H_{L_{OUT}}L_{OUT} + H_{V_{OUT}}V_{OUT}$	1
Mole fraction constraints, e.g. $\sum_{i=1}^{C}(x_i)_{L_{IN}} = 1.0$	4
	$N_E = 2C + 7$

Alternatively, C component material balances can be written. The total material balance is then a dependent equation obtained by summing the component material balances and applying the mole fraction constraints to eliminate the mole fractions. From (6-1)

$$N_D = (4C + 12) - (2C + 7) = 2C + 5$$

Several different sets of design variables can be specified. A typical set includes complete specification of the two entering streams as well as the stage pressure.

Variable Specification	Number of Variables
Component mole fractions, $(x_i)_{L_{IN}}$	$C-1$
Total flow rate, L_{IN}	1
Component mole fractions, $(y_i)_{V_{IN}}$	$C-1$
Total flow rate, V_{IN}	1
Temperature and pressure of L_{IN}	2
Temperature and pressure of V_{IN}	2
Stage pressure ($P_{V_{OUT}}$ or $P_{L_{OUT}}$)	1
	$N_D = 2C+5$

Specification of these $(2C+5)$ variables permits calculation of the unknown variables L_{OUT}, V_{OUT}, $(x_C)_{L_{IN}}$, $(y_C)_{V_{IN}}$, all $(x_i)_{L_{OUT}}$, T_{OUT}, and all $(y_i)_{V_{OUT}}$, where C denotes the missing mole fraction.

6.3 Equilibrium Stage with Heat Addition, Feed Stream, and Sidestream

A more complex equilibrium stage is shown in Fig. 6.2. The feed stream has no variable values in common with L_{IN} and V_{OUT}, but the liquid side stream shown leaving the stage is identical in composition, T, and P to L_{OUT} though different in flow rate. Heat can be transferred to or from the stage at the rate Q (where a positive value denotes addition of heat to the stage). The number of total variables (including Q) is

$$N_V = 6(C+3)+1 = 6C+19$$

The equations for this element are similar to those for an adiabatic equilibrium stage. But, in addition, component mole fractions of L_{OUT} and side stream S are identical. This situation is handled by $C-1$ mole fraction equalities with the missing mole fractions accounted for by the usual mole fraction constraints.

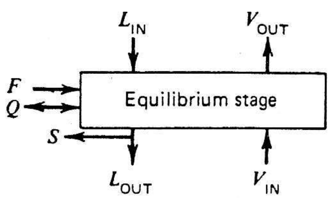


Figure 6.2. Equilibrium stage with heat addition, feed, and side stream.

Equations	Number of Equations
Pressure equalities, $P_{V_{OUT}} = P_{L_{OUT}} = P_S$	2
Temperature equalities, $T_{V_{OUT}} = T_{L_{OUT}} = T_S$	2
Phase equilibrium relationships, $(y_i)_{V_{OUT}} = K_i(x_i)_{L_{OUT}}$	C
Component material balances, $L_{IN}(x_i)_{L_{IN}} + V_{IN}(y_i)_{V_{IN}} + F(x_i)_F = L_{OUT}(x_i)_{L_{OUT}} + S(x_i)_S + V_{OUT}(y_i)_{V_{OUT}}$	$C-1$
Total material balance, $F + L_{IN} + V_{IN} = L_{OUT} + S + V_{OUT}$	1
Enthalpy balance, $H_F F + H_{L_{IN}} L_{IN} + H_{V_{IN}} V_{IN} + Q = H_{L_{OUT}} L_{OUT} + H_S S + H_{V_{OUT}} V_{OUT}$	1
Mole fraction constraints, e.g. $\sum_{i=1}^{C} (x_i)_S = 1.0$	6
Mole fraction equalities, $(x_i)_{L_{OUT}} = (x_i)_S$	$C-1$
	$N_E = 3C + 10$

From (6-1)

$$N_D = (6C + 19) - (3C + 10) = 3C + 9$$

A typical set of design variables is as follows. Many other sets are possible.

Variable Specification	Number of Variables
Component mole fractions, $(x_i)_{L_{IN}}$	$C-1$
Total flow rate, L_{IN}	1
Component mole fractions, $(y_i)_{V_{IN}}$	$C-1$
Total flow rate, V_{IN}	1
Component mole fractions, $(x_i)_F$	$C-1$
Total flow rate, F	1
T and P of L_{IN}, V_{IN}, F	6
Stage pressure ($P_{V_{OUT}}$, $P_{L_{OUT}}$, or P_S)	1
Stage temperature ($T_{V_{OUT}}$, $T_{L_{OUT}}$, or T_S)	1
Total side stream flow rate, S	1
	$3C+9$

These specifications differ from those given previously for an adiabatic stage in that the required heat transfer rate is an output variable. Alternatively, the heat transfer rate Q can be specified with stage temperature treated as an output variable. Also, an algebraic combination of variables can be specified in place of a single variable—for example, a value for S/L_{OUT} instead of a value for the total side stream flow rate S.

6.4 Condenser and Boiler

Figure 6.3 shows a boiler; if the flows of heat and mass are reversed, it is a condenser. Complete vaporization or condensation is assumed. The number of variables is

$$N_V = 2(C+3)+1 = 2C+7$$

The equations are

Equations	Number of Equations
Component material balances	$C-1$
Total material balance	1
Enthalpy balance	1
Mole fraction constraints	2
	$N_E = C+3$

The degrees of freedom are

$$N_D = (2C+7)-(C+3) = C+4$$

By specifying, for example, $C-1$ input flow component mole fractions, the total input flow rate, and T and P of both output and input streams, one can calculate Q.

If only partial condensation or vaporization occurs, equipment schematic diagrams are as shown in Fig. 6.4*a* and 6.4*b*.

The analysis for either element is identical. The total variables equal

$$N_V = 3(C+3)+1 = 3C+10$$

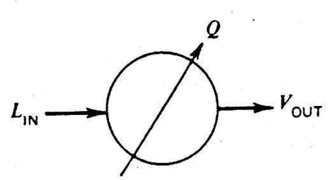


Figure 6.3. Boiler.

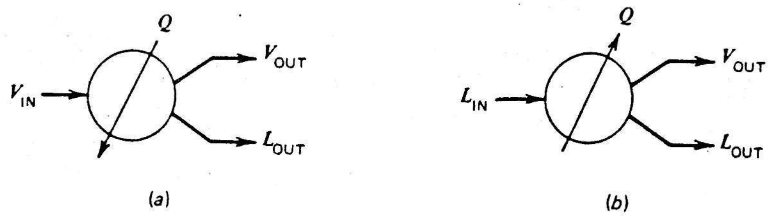


Figure 6.4. Partial condenser and vaporizer. (*a*) Partial condenser, (*b*) Partial vaporizer.

Relations among the variables include the following, where V_{OUT} and L_{OUT} are in equilibrium.

Equations	**Number of Equations**
Component material balances	$C-1$
Total material balance	1
Enthalpy balance	1
Pressure equality, $P_{V_{OUT}} = P_{L_{OUT}}$	1
Temperature equality, $T_{V_{OUT}} = T_{L_{OUT}}$	1
Phase equilibrium relationships, $(y_i)_{V_{OUT}} = K_i(x_i)_{L_{OUT}}$	C
Mole fraction constraints	3
	$N_E = 2C + 6$

Thus $N_D = C + 4$, which is identical to the result obtained for the total condenser or boiler.

6.5 Mixer, Divider, and Splitter

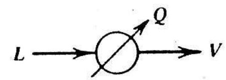
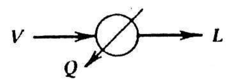
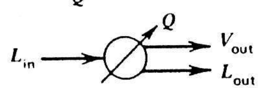
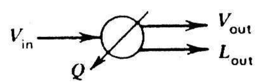
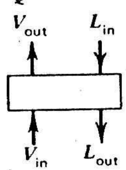
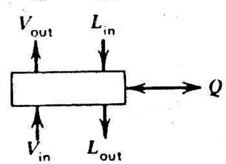
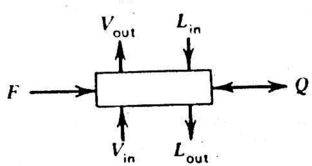
For mixers, dividers, and splitters involving three streams, as shown in Fig. 6.5, $N_V = 3(C+3)+1 = 3C+10$. Equations for the mixer include $(C-1)$ component material balances, a total material balance, an enthalpy balance, and three mole fraction constraints.

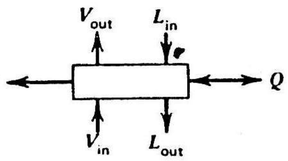
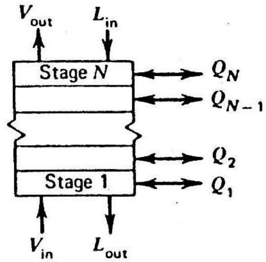
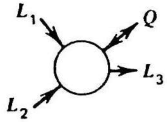
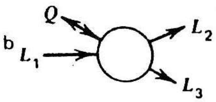
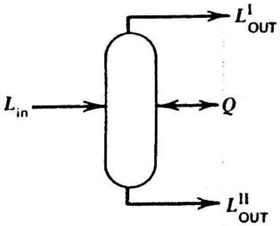
$$N_D = 3(C+3) + 1 - (C+4) = 2C + 6$$

Typical variable specifications are feed conditions for both inlet streams ($2C+4$ variables), outlet stream pressure, and Q. All three streams are assumed to be of the same phase state (vapor or liquid).

In the stream divider, the relations include $[2(C-1)]$ mole fraction equalities because all three streams have the same composition. There are also

Table 6.1 Degrees of freedom for separation operation elements and units

Schematic	Element or Unit Name	N_V, Total Variables	N_E, Independent Relationships	N_D, Degrees of Freedom
	Total boiler (Reboiler)	$(2C+7)$	$(C+3)$	$(C+4)$
	Total condenser	$(2C+7)$	$(C+3)$	$(C+4)$
	Partial (equilibrium) boiler (reboiler)	$(3C+10)$	$(2C+6)$	$(C+4)$
	Partial (equilibrium) condenser	$(3C+10)$	$(2C+6)$	$(C+4)$
	Adiabatic equilibrium stage	$(4C+12)$	$(2C+7)$	$(2C+5)$
	Equilibrium stage with heat transfer	$(4C+13)$	$(2C+7)$	$(2C+6)$
	Equilibrium feed stage with heat transfer and feed	$(5C+16)$	$(2C+8)$	$(3C+8)$

[a] 	Equilibrium stage with heat transfer and side stream	$(5C + 16)$	$(3C + 9)$	$(2C + 7)$
	N connected equilibrium stages with heat transfer	$(7N + 2NC + 2C + 7)$	$(5N + 2NC + 2)$	$(2N + 2C + 5)$
	Stream mixer	$(3C + 10)$	$(C + 4)$	$(2C + 6)$
[b] 	Stream divider	$(3C + 10)$	$(2C + 5)$	$(C + 5)$
[c] 	Splitter, composition of $L^{II}_{OUT} \neq L^{I}_{OUT}$	$(3C + 10)$	$(C + 4)$	$(2C + 6)$

[a] Side stream can be vapor or liquid. [b] Alternatively, all streams can be vapor. [c] Any stream can be vapor.

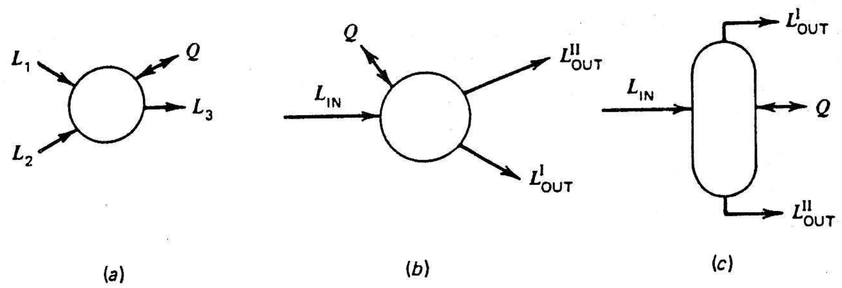


Figure 6.5. Mixer, divider and splitter. (*a*) Mixer. (*b*) Divider. (*c*) Splitter.

pressure and temperature identities between L^{II}_{OUT} and L^{I}_{OUT}, plus one total material balance, one enthalpy balance, and three mole fraction constraints. Thus

$$N_D = (3C + 10) - (2C + 5) = C + 5$$

Variable specifications for the stream divider are typically $(C + 2)$ feed variables, outlet temperature (or heat transfer rate) and outlet pressure, and L^{II}_{OUT}, L^{I}_{OUT}/L^{II}_{OUT}, L^{I}_{OUT}/L_{IN}, and so on.

In the splitter, composition of L^{I}_{OUT} is not equal to L^{II}_{OUT} or L_{IN}. Also, stream compositions are not related by equilibrium constraints, nor need the outlet streams be at the same temperature or pressure. Thus, the only relationships are $(C - 1)$ component balances, one total material balance, an enthalpy balance, and three mole fraction constraints, so that

$$N_D = (3C + 10) - (C + 4) = 2C + 6$$

Examples of splitters are devices in which nonequilibrium separations are achieved by means of membranes, electrical fields, temperature changes, and others. The splitter can also be used to model any multistage chemical separator where stage details are not of interest.

Table 6.1 is a summary of the degrees of freedom in representative building-block elements for separation operations.

6.6 Combinations of Elements by an Enumeration Algorithm

An algorithm is easily developed for enumerating variables, equations, and degrees of freedom for combinations of elements to form units. The number of design variables for a separator (e.g., a distillation column) is obtained by summing the variables associated with the individual equilibrium stages, heat exchangers, and other elements e that comprise the separator. However, care must be taken to subtract from the total variables the $(C+3)$ variables for each of the N_R redundant interconnecting streams that arise when the output of one process element becomes the input to another. Also, if an unspecified number of repetitions of any element occurs within the unit, an additional variable is added, one for each group of repetitions, giving a total of N_A additional variables. In addition, N_R redundant mole fraction constraints are subtracted after summing the independent relationships of the individual elements. The number of degrees of freedom is obtained as before, from (6-1). Thus

$$(N_V)_{\text{unit}} = \sum_{\substack{\text{all} \\ \text{elements, } e}} (N_V)_e - N_R(C+3) + N_A \qquad (6\text{-}2)$$

$$(N_E)_{\text{unit}} = \sum_{\substack{\text{all} \\ \text{elements, } e}} (N_E)_e - N_R \qquad (6\text{-}3)$$

Combining (6-1), (6-2), and (6-3), we have

$$(N_D)_{\text{unit}} = \sum_{\substack{\text{all} \\ \text{elements, } e}} (N_D)_e - N_R(C+2) + N_A \qquad (6\text{-}4)$$

or

$$(N_D)_{\text{unit}} = (N_V)_{\text{unit}} - (N_E)_{\text{unit}} \qquad (6\text{-}5)$$

For the N-stage cascade unit of Fig. 6.6, with reference to the single

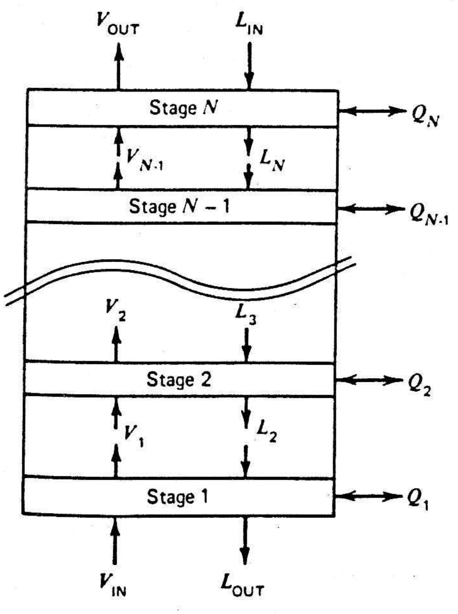


Figure 6.6. An N-stage cascade.

equilibrium stage with heat transfer in Table 6.1, the total variables from (6-2) are

$$(N_V)_{\text{unit}} = N(4C+13) - [2(N-1)](C+3) + 1 = 7N + 2NC + 2C + 7$$

since $2(N-1)$ interconnecting streams exist. The additional variable is the total number of stages (i.e., $N_A = 1$).

The number of independent relationships from (6-3) is

$$(N_E)_{\text{unit}} = N(2C+7) - 2(N-1) = 5N + 2NC + 2$$

since $2(N-1)$ redundant mole fraction constraints exist.

The degrees of freedom from (6-5) are

$$(N_D)_{\text{unit}} = N_V - N_E = 2N + 2C + 5$$

One possible set of design variables is

Variable Specification	Number of Variables
Heat transfer rate for each stage (or adiabaticity)	N
Stage pressures	N
Stream V_{IN} variables	$C+2$
Stream L_{IN} variables	$C+2$
Number of stages	1
	$2N+2C+5$

Output variables for this specification include missing mole fractions for V_{IN} and L_{IN}, stage temperatures, and the variables associated with the V_{OUT} stream, L_{OUT} stream, and interstage streams. The results obtained in this example are included in Table 6.1. The N-stage cascade unit can represent simple absorbers, strippers, or liquid–liquid extractors.

6.7 Description Rule

An attractive alternative to counting variables and equations is to use the *Description Rule* of Hanson, Duffin, and Somerville.[2]

> To completely describe the separation operation, the number of independent variables which must be set, must equal the number that can be set by construction or controlled by external means.

To apply this rule it is necessary to identify the variables that "can be set by construction or controlled by external means." For the cascade shown in Fig.

6.6, this is easily done. They are

Variable	Number of Variables
Stage pressure	N
Stage temperature (or Q)	N
Feed stream V_{IN} variables	$C+2$
Feed stream L_{IN} variables	$C+2$
Number of stages	1
	$N_D = 2N + 2C + 5$

This is in agreement with the results obtained by enumeration.

6.8 Complex Units

In applying either the Description Rule of Section 6.7 or the enumeration algorithm of Section 6.6 to complex multistage separators that have auxiliary heat exchangers, boilers, stream mixers, stream dividers, and so on, a considerable amount of physical insight is required to develop a feasible list of design variables. This can best be illustrated by a few examples.

Example 6.1 Consider a multistage distillation column with one feed, one side stream, total condenser, partial reboiler, and provisions for heat transfer to or from any stage. This separator can be composed, as shown in Fig. 6.7, from the circled elements and units. Total variables are determined from (6-2) by summing the variables $(N_V)_e$ for each unit from Table 6.1 and then subtracting the redundant variables due to interconnecting flows. As before, redundant mole fraction constraints are subtracted from the summation of independent relationships for each element $(N_E)_e$. This problem was first treated by Gilliland and Reed[3] and more recently by Kwauk[1] and Smith.[4] Differences in N_D obtained by various authors are due, in part, to their method of numbering stages.

Solution. Here, the partial reboiler is the first equilibrium stage. From Table 6.1, element variables and relationships are obtained as follows.

Element or Unit	$(N_V)_e$	$(N_E)_e$
Total condenser	$(2C+7)$	$(C+3)$
Reflux divider	$(3C+10)$	$(2C+5)$
$(N-S)$ stages	$[7(N-S)+2(N-S)C+2C+7]$	$[5(N-S)+2(N-S)C+2]$
Side-stream stage	$(5C+16)$	$(3C+9)$
$(S-1)-(F)$ stages	$[7(S-1-F)+2(S-1-F)C+2C+7]$	$[5(S-1-F)+2(S-1-F)C+2]$
Feed stage	$(5C+16)$	$(2C+8)$
$(F-1)-1$ stages	$[7(F-2)+2(F-2)C+2C+7]$	$[5(F-2)+2(F-2)C+2]$
Partial reboiler	$(3C+10)$	$(2C+6)$
	$\Sigma (N_V)_e = 7N + 2NC + 18C + 59$	$\Sigma (N_E)_e = 5N + 2NC + 4C + 22$

Subtracting $(C+3)$ redundant variables for 13 interconnecting streams, according to (6-2) with $N_A = 0$ (no unspecified repetitions) gives

$$(N_V)_{\text{unit}} = \sum (N_V)_e - 13(C+3) = 7N + 2NC + 5C + 20$$

Subtracting the corresponding 13 redundant mole fraction constraints, according to (6-3), we have

$$(N_E)_{\text{unit}} = \sum (N_E)_e - 13 = 5N + 2NC + 4C + 9$$

Therefore, from (6-5)

$$N_D = (7N + 2NC + 5C + 20) - (5N + 2NC + 4C + 9) = 2N + C + 11$$

A set of feasible design variable specifications is

Variable Specification	*Number of Variables*
1. Pressure at each stage (including partial reboiler)	N
2. Pressure at reflux divider outlet	1
3. Pressure at total condenser outlet	1
4. Heat transfer rate for each stage (excluding partial reboiler)	$(N-1)$
5. Heat transfer rate for divider	1
6. Feed mole fractions and total feed rate	C
7. Feed temperature	1
8. Feed pressure	1
9. Condensate temperature (e.g., saturated liquid)	1
10. Total number of stages N	1
11. Feed stage location	1
12. Side-stream stage location	1
13. Side-stream total flow rate S	1
14. Total distillate flow rate, D or D/F	1
15. Reflux flow rate L_R or reflux ratio L_R/D	1
	$N_D = (2N + C + 11)$

In most separation operations, variables related to feed conditions, stage heat transfer rates, and stage pressures are known or set. Remaining specifications have proxies, provided that the variables are mathematically independent of each other and of those already known. Thus, in the above list the first 9 entries are almost always known or specified. Variables 10 to 15, however, have surrogates. Some of these are:

16. Condenser heat duty Q_C
17. Reboiler heat duty Q_R
18. Recovery or mole fraction of one component in bottoms
19. Recovery or mole fraction of one component in distillate
20. Maximum vapor rate in column

The combination 1 to 9, 10, 11, 12, 14, 16, and 20 is convenient if the problem is one of calculating the performance of an existing column on a new feed. Here the maximum vapor rate is known as is the condenser heat duty, and the product compositions are calculated.

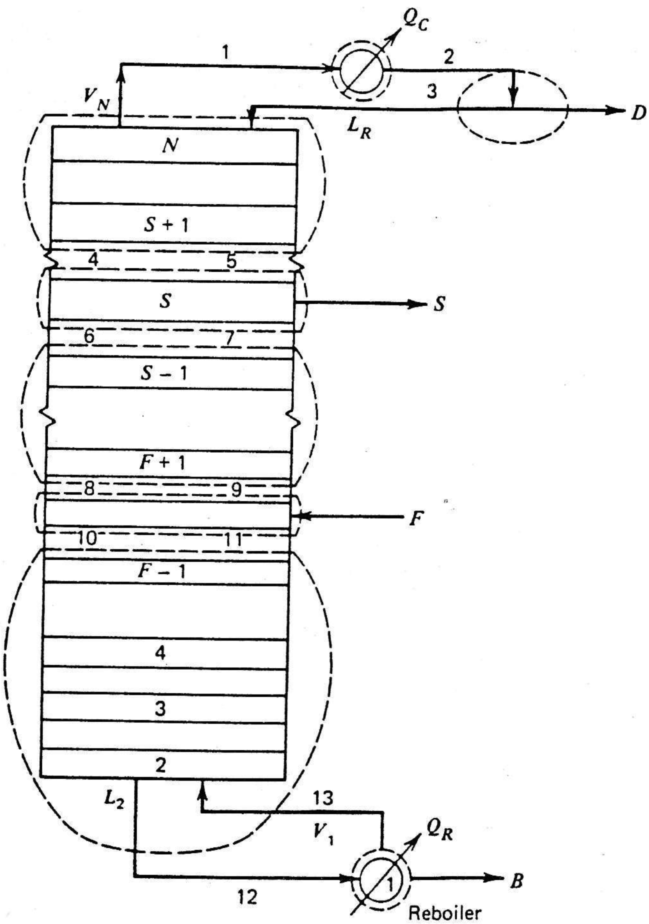


Figure 6.7. Complex distillation unit.

Heat duties Q_C and Q_R are not good design variables because they are difficult to specify. Condenser duty Q_C, for example, must be specified so that the condensate temperature lies between that corresponding to a saturated liquid and the freezing point of the condensate. Otherwise, a physically unrealizable (or no) solution to the problem is obtained. Similarly, it is much easier to calculate Q_R knowing the total flow rate and enthalpy of the bottom streams than vice versa. In general Q_R and the maximum vapor rate are so closely related that it is not advisable to specify both of them. The same is true of Q_C and Q_R.

Other proxies are possible—stage temperatures, for example, or a flow for each stage, or any independent variable that characterizes the process. The problem of independence of variables requires careful consideration. Distillate product rate, Q_C, and L_R/D, for example, are not independent. It should be noted also that, for the design case, we specify recoveries of no more than two species (items 18 and 19). These species are referred to as key components. Attempts to specify recoveries of three or four species will usually result in unsuccessful solutions of the equations.

□

Example 6.2. Consider a liquid–liquid extraction separator with central feed and extract reflux, as shown in Fig. 6.8. The five elements or units circled are a set of stages above the feed stage, the feed stage, a set of stages below the feed stage, the splitter, in which solvent is recovered, and a divider that sends reflux to the bottom stage. Suggest a feasible set of design variables.

Solution. The degrees of freedom for this complex separator unit can be determined as in Example 6.1. An alternative method is to apply (6-4) by summing the degrees of freedom for each element $(N_D)_e$ and subtracting $(C+2)$ redundant independent variables for each interconnecting stream. Using this alternative procedure with values of $(N_D)_e$ from Table 6.1, the elements and design variables are:

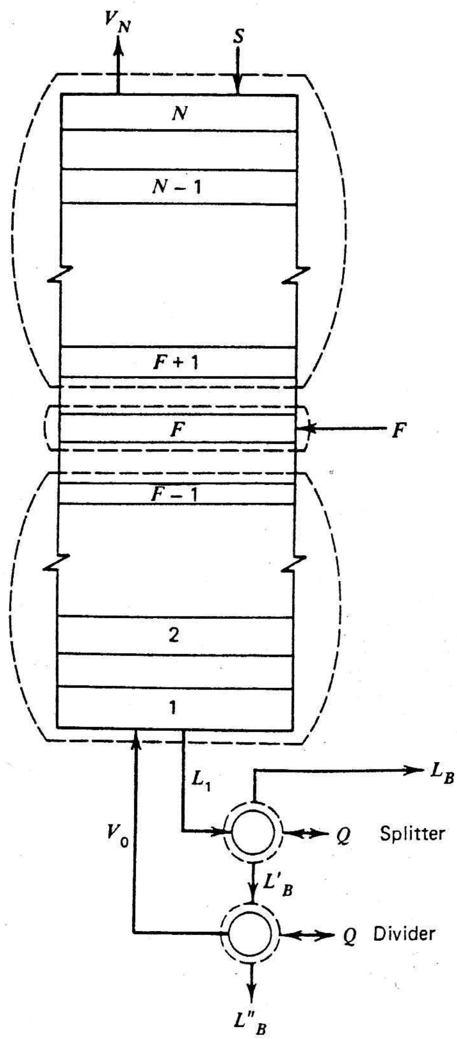


Figure 6.8. Liquid–liquid extraction unit.

Element	$(N_D)_e$
$(N-F)$ stages	$[2(N-F)+2C+5]$
Feed stage	$(3C+8)$
$(F-1)$ stages	$[2(F-1)+2C+5]$
Splitter	$(2C+6)$
Divider	$(C+5)$
	$\Sigma\,(N_D)_e=(2N+10C+27)$

There are seven interconnecting streams. Thus, the number of design variables from (6-4) is:

$$(N_D)_{\text{unit}}=(2N+10C+27)-7(C+2)$$
$$=2N+3C+13$$

A feasible set of variable specifications is:

Variable Specification	*Number of Variables*
Pressure at each stage	N
Temperature or heat transfer rate for each stage	N
Solvent feed flow rate, composition, temperature, and pressure	$(C+2)$
Feed stream flow rate, composition, temperature, and pressure	$(C+2)$
Total number of stages N	1
Feed stage location	1
Splitter:	
Component recovery	C
T, P of L_B and L'_B	4
Divider:	
P, Q	2
Reflux ratio, V_0/L''_B	1
	$N_D=2N=3C+13$

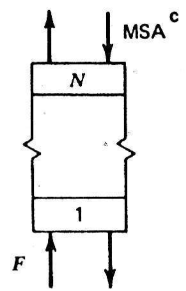
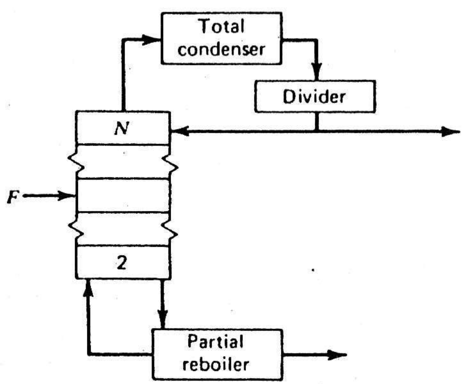
□

Example 6.3. Is the following problem from Henley and Staffin[5] completely specified?

> A mixture of maleic anhydride and benzoic acid containing 10 mole percent acid is a product of the manufacture of phthalic anhydride. The mixture is to be distilled continuously at a pressure of 13.2 kPa [100 torr] to give a product of 99.5 mole percent maleic anhydride and a bottoms of 0.5 mole percent anhydride. Using the data below [omitted here], calculate the number of plates (stages) using an L/D of 1.6 times the minimum.

Solution. The degrees of freedom for this distillation operation are determined as follows by using Table 6.1, assuming the partial reboiler is the first stage.

Table 6.2 Typical variable specifications for design cases

Unit Operation		N_D	Variable Specification[a]: Case I, Component Recoveries Specified	Variable Specification[a]: Case II, Number of Equilibrium Stages Specified
(*a*) Absorption (two inlet streams)		$2N+2C+5$	1. Recovery of one key component.	1. Number of stages.
(*b*) Distillation (one inlet stream, total condenser, partial reboiler)		$2N+C+9$	1. Condensate at saturation temperature. 2. Recovery of light-key component. 3. Recovery of heavy-key component. 4. Reflux ratio (> minimum). 5. Optimum feed stage.[b]	1. Condensate at saturation temperature. 2. Number of stages above feed stage. 3. Number of stages below feed stage. 4. Reflux ratio. 5. Distillate flow rate.

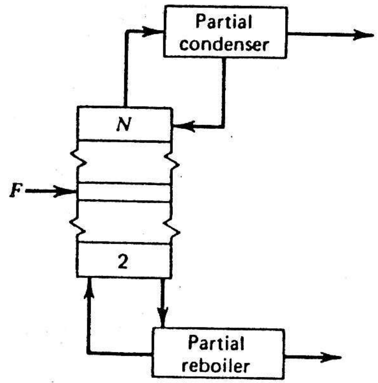
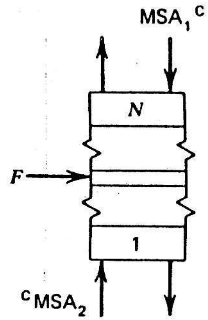
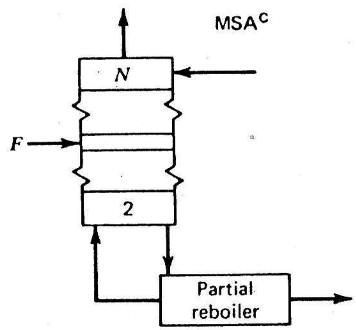
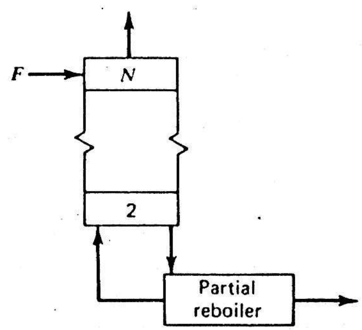
(*c*) Distillation (one inlet stream, partial condenser, partial reboiler, vapor distillate only)		$2N + C + 6$	1. Recovery of light-key component. 2. Recovery of heavy-key component. 3. Reflux ratio (> minimum). 4. Optimum feed stage.[b]	1. Number of stages above feed stage. 2. Number of stages below feed stage. 3. Reflux ratio. 4. Distillate flow rate.
(*d*) Liquid–liquid extraction with two solvents (three inlet streams)		$2N + 3C + 8$	1. Recovery of key component one. 2. Recovery of key component two.	1. Number of stages above feed. 2. Number of stages below feed.

Table 6.2, continued

Unit Operation		N_D	Variable Specification[a]: Case I, Component Recoveries Specified	Variable Specification[a]: Case II, Number of Equilibrium Stages Specified
(*e*) Reboiled absorption (two inlet streams)		$2N+2C+6$	1. Recovery of light-key component. 2. Recovery of heavy-key component. 3. Optimum feed stage.[b]	1. Number of stages above feed. 2. Number of stages below feed. 3. Bottoms flow rate.
(*f*) Reboiled stripping (one inlet stream)		$2N+C+3$	1. Recovery of one key component. 2. Reboiler heat duty.[d]	1. Number of stages. 2. Bottoms flow rate.

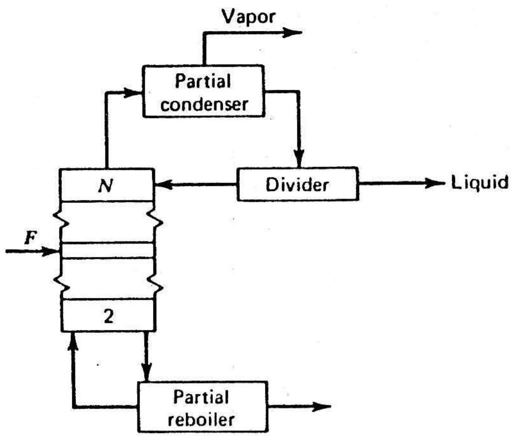
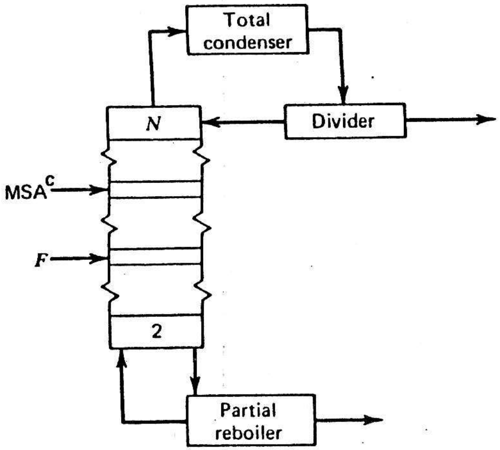
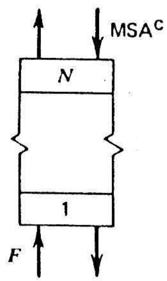
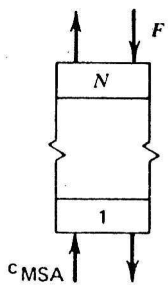
(*g*) Distillation (one inlet stream, partial condenser, partial reboiler, both liquid and vapor distillates)		$2N + C + 9$	1. Ratio of vapor distillate to liquid distillate. 2. Recovery of light-key component. 3. Recovery of heavy-key component. 4. Reflux ratio (> minimum). 5. Optimum feed stage.[b]	1. Ratio of vapor distillate to liquid distillate. 2. Number of stages above feed stage. 3. Number of stages below feed stage. 4. Reflux ratio. 5. Liquid distillate flow rate.
(*h*) Extractive distillation (two inlet streams, total condenser, partial reboiler, single-phase condensate)		$2N + 2C + 12$	1. Condensate at saturation temperature. 2. Recovery of light-key component. 3. Recovery of heavy-key component. 4. Reflux ratio (> minimum) 5. Optimum feed stage.[b] 6. Optimum MSA stage.[b]	1. Condensate at saturation temperature. 2. Number of stages above MSA stage. 3. Number of stages between MSA and feed stages. 4. Number of stages below feed stage. 5. Reflux ratio. 6. Distillate flow rate.

Table 6.2, continued

Unit Operation		N_D	Variable Specification[a] Case I, Component Recoveries Specified	Variable Specification[a] Case II, Number of Equilibrium Stages Specified
(*i*) Liquid–liquid extraction (two inlet streams)		$2N + 2C + 5$	1. Recovery of one key component.	1. Number of stages.
(*j*) Stripping (two inlet streams)		$2N + 2C + 5$	1. Recovery of one key component.	1. Number of stages.

[a] Does not include the following variables, which are also assumed specified: all inlet stream variables ($C + 2$ for each stream); all element and unit pressures; all element and unit heat transfer rates except for condensers and reboilers.
[b] Optimum stage for introduction of inlet stream corresponds to minimization of total stages.
[c] For Case I variable specifications, MSA flow rates must be greater than minimum values for specified recoveries.
[d] For Case I variable specifications, reboiler heat duty must be greater than minimum value for specified recovery.

Element or Unit	$(N_D)_e$
Reflux divider	$(C+5)$
Total condenser	$(C+4)$
Stages above feed stage	$[2(N-F)+2C+5]$
Stages below feed stage	$[2(F-2)+2C+5]$
Feed stage	$(3C+8)$
Partial reboiler	$(C+4)$
	$\Sigma (N_D)_e = 2N+10C+27$

There are nine interconnecting streams. Thus, the degrees of freedom from (6-4) are

$$N_D = 2N + 10C + 27 - 9(C+2) = 2N + C + 9$$

The only variables specified in the problem statement are

Variable Specification	*Number of Variables*
Stage pressures (including reboiler)	N
Condenser pressure	1
Reflux divider pressure	1
L_R/D	1
Feed composition	$C-1$
Mole fraction of maleic anhydride in distillate	1
Mole fraction of maleic anhydride in bottoms	1
	$C+N+4$

The problem is underspecified by $(N+5)$ variables. It can be solved if we assume:

Additional Variable Specification	*Number of Variables*
Feed T and P	2
Total condenser giving saturated reflux	1
Heat transfer rate (loss) in divider	1
Adiabatic stages (excluding boiler, which is assumed to be a partial reboiler	$N-1$
Feed stage location (assumed to be optimum)	1
Feed rate	1
	$N+5$

□

6.9 Variable Specifications for Typical Design Cases

The design of multistage separation operations involves solving the variable relationships for output variables after selecting values of design variables to satisfy the degrees of freedom. Two cases are commonly encountered. In Case I, recovery specifications are made for one or two key components and the number of required equilibrium stages is determined. In Case II, the number of equilibrium stages is specified and component separations are computed. For multicomponent feeds, the second case is more widely employed because less computational complexity is involved. Table 6.2 is a summary of possible variable specifications for each of these two cases for a number of separator types previously discussed in Chapter 1 and shown in Table 1.1. For all separators in Table 6.2, it is assumed that all inlet streams are completely specified (i.e., $C-1$ mole fractions, total flow rate, temperature, and pressure) and all element and unit pressures and heat transfer rates (except for condensers and reboilers) are specified. Thus, only variables to satisfy the remaining degrees of freedom are listed.

References

1. Kwauk, M., *AIChE J.*, **2**, 240–248 (1956).
2. Hanson, D. N., J. H. Duffin, and G. F. Somerville, *Computation of Multistage Separation Processes*, Reinhold Publishing Corporation, New York, 1962, Chapter 1.
3. Gilliland, E. R., and C. E. Reed, *Ind. Eng. Chem.*, **34**, 551–557 (1942).
4. Smith, B., *Design of Equilibrium Stage Processes*, McGraw–Hill Book Co., New York, 1963, Chapter 3.
5. Henley, E. J., and H. K. Staffin, *Stagewise Process Design*, John Wiley & Sons, Inc., New York, 1963, 198.

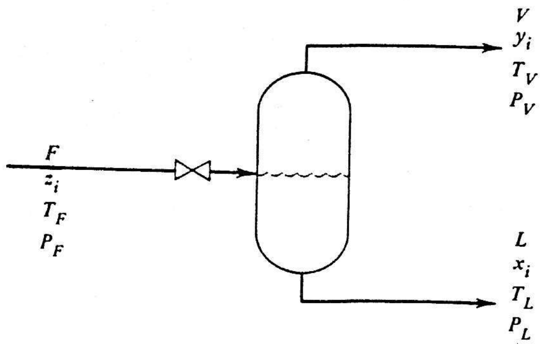
Problems

6.1 Consider the equilibrium stage shown in Fig. 1.12. Conduct a degrees-of-freedom analysis by performing the following steps.
(a) List and count the variables.
(b) Write and count the equations relating the variables.
(c) Calculate the degrees of freedom.
(d) List a reasonable set of design variables.

6.2 Can the following problems be solved uniquely?
(a) The feed streams to an adiabatic equilibrium stage consist of liquid and vapor streams of known composition, flow rate, temperature, and pressure. Given the stage (outlet) temperature and pressure, calculate the composition and amounts of equilibrium vapor and liquid leaving the stage.
(b) The same as Part (a), except that the stage is not adiabatic.
(c) The same as Part (a), except that, in addition to the vapor and liquid streams leaving the stage, a vapor side stream, in equilibrium with the vapor leaving the stage, is withdrawn.
(d) A multicomponent vapor of known temperature, pressure, and composition is to be partially condensed in a condenser. The pressure in the condenser and the inlet cooling water temperature are fixed. Calculate the cooling water required.
(e) A mixture of ^{235}U and ^{238}U is partially diffused through a porous membrane

barrier to effect isotope enrichment. The process is adiabatic. Given the separation factor and the composition and conditions of the feed, calculate the pumping requirement.

6.3 Consider an adiabatic equilibrium flash. The variables are all as indicated in the sketch below.



(a) Determine N_v = number of variables.
(b) Write all the independent equations that relate the variables.
(c) Determine N_E = number of equations.
(d) Determine the number of degrees of freedom.
(e) What variables would you prefer to specify in order to solve a typical adiabatic flash problem?

6.4 Determine the number of degrees of freedom for a nonadiabatic equilibrium flash for one liquid feed, one vapor stream product, and two immiscible liquid stream products.

6.5 Determine N_D for the following unit operations in Table 6.2: (*b*), (*c*), and (*g*).

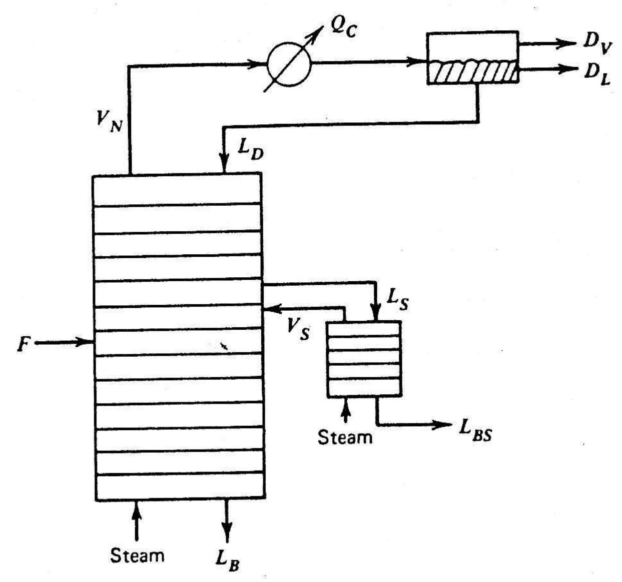
6.6 Determine N_D for unit operations (*e*) and (*f*) in Table 6.2.

6.7 Determine N_D for unit operation (*h*) in Table 6.2. How would N_D change if a liquid side stream were added to a stage that was located between the feed *F* and stage 2?

6.8 The following are not listed as design variables for the distillation unit operations in Table 6.2.
(a) Condenser heat duty.
(b) Stage temperature.
(c) Intermediate stage vapor rate.
(d) Reboiler heat load.
Under what conditions might these become design variables? If so, which variables listed in Table 6.2 would you eliminate?

6.9 Show for distillation that, if a total condenser is replaced by a partial condenser, the degrees of freedom are reduced by three, provided that the distillate is removed solely as a vapor.

6.10 Determine the number of independent variables and suggest a reasonable set for (a) a new column, and (b) an existing column, for the crude oil distillation column with side stripper shown below. Assume that water does not condense.



6.11 Show that the degrees of freedom for a liquid–liquid extraction column with two feeds and raffinate reflux is $3C + 2N + 13$.

6.12 Determine the degrees of freedom and a reasonable set of specifications for an azeotropic distillation problem wherein the formation of one minimum-boiling azeotrope occurs.

6.13 A distillation column consisting of four equilibrium trays, a reboiler, a partial condenser, and a reflux divider is being used to effect a separation of a five-component stream.

The feed is to the second tray, the trays and divider are adiabatic, and the pressure is fixed throughout the column. The feed is specified.

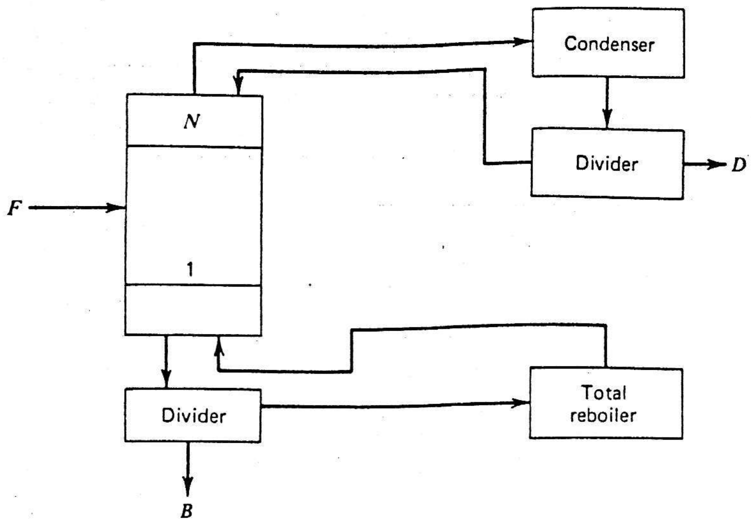
The control engineer has specified three control loops that he believes to be independent. One is to control the reflux/distillate ratio, the second to control the distillate/feed ratio, and the third to maintain top tray temperature. Comment on this proposed control scheme.

6.14 (a) Determine for the distillation column below the number of independent design variables.

(b) It is suggested that a feed consisting of 30% A, 20% B, and 50% C at 37.8°C and 689 kPa be processed in an existing 15-plate, 3-m-diameter column that is designed to operate at vapor velocities of 0.3 m/sec and an L/V of 1.2. The pressure drop per plate is 373 Pa at these conditions, and the condenser is cooled by plant water, which is at 15.6°C.

The product specifications in terms of the concentration of A in the distillate and C in the bottoms have been set by the process department, and the plant manager has asked you to specify a feed rate for the column.

Write a memorandum to the plant manager pointing out why you can't do this and suggest some alternatives.



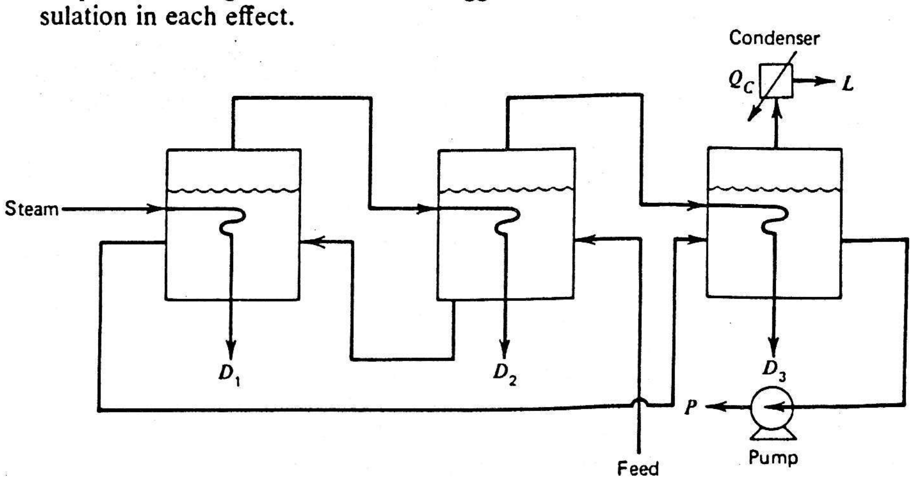
6.15 Unit operation (*b*) in Table 6.2 is to be heated by injecting live steam directly into the bottom plate of the column instead of by using a reboiler, for a separation involving ethanol and water. Assuming a fixed feed, an adiabatic operation, atmospheric pressure throughout, and a top alcohol concentration specification:

(a) What is the total number of design variables for the general configuration?

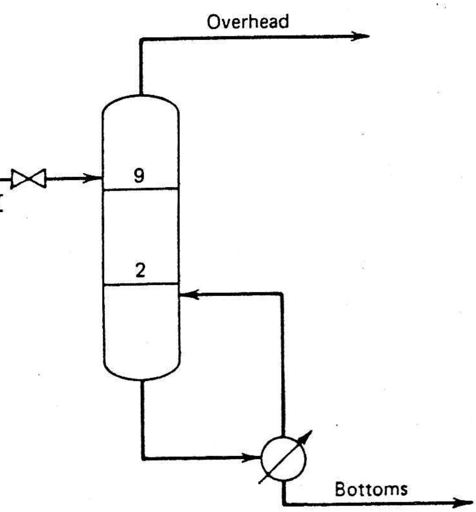
(b) How many design variables will complete the design? Which variables do you recommend?

6.16 Calculate the degrees of freedom of the mixed-feed triple-effect evaporator shown below. Assume the steam and all drain streams are at saturated conditions and the feed is an aqueous solution of dissolved organic solids (two-component streams). Also, assume that all overhead streams are pure water vapor with no entrained solids (one-component streams).

If this evaporator is used to concentrate a feed containing 2% solids to a product with 25% solids using 689 kPa saturated steam, calculate the number of unspecified design variables and suggest likely candidates. Assume perfect insulation in each effect.



6.17 A reboiled stripper is to be designed for the task shown below. Determine:
(a) The number of variables.
(b) The number of equations relating the variables.
(c) The number of degrees of freedom.
and indicate:
(d) Which additional variables, if any, need to be specified.



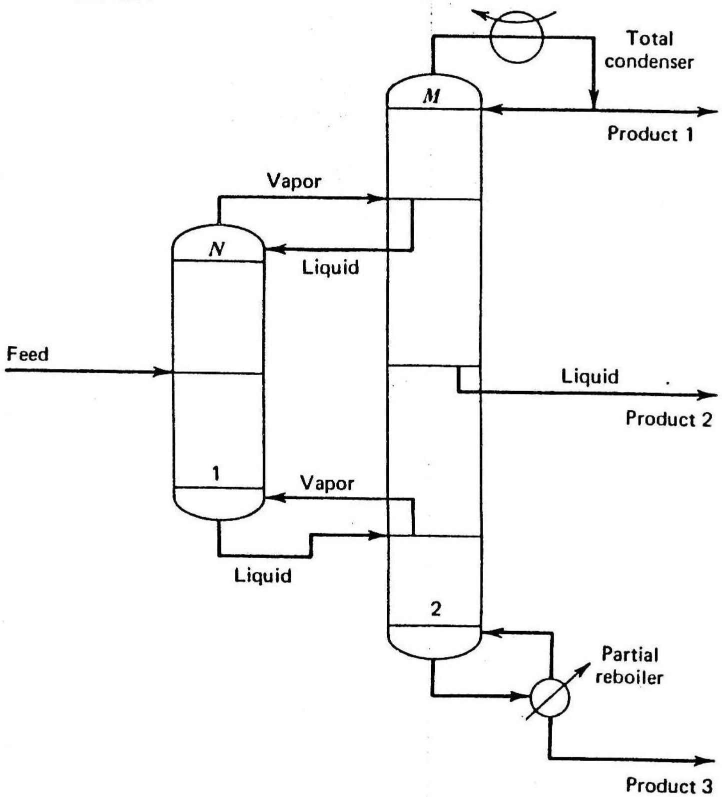
Comp.	Kgmole/hr
N_2	1.0
C_1	54.4
C_2	67.6
C_3	141.1
C_4	154.7
C_5	56.0
C_6	33.3

6.18 The thermally coupled distillation system shown below is to be used to separate a mixture of three components into three products. Determine for the system:
(a) The number of variables.
(b) The number of equations relating the variables.
(c) The number of degrees of freedom.
and propose:
(d) A reasonable set of design variables.

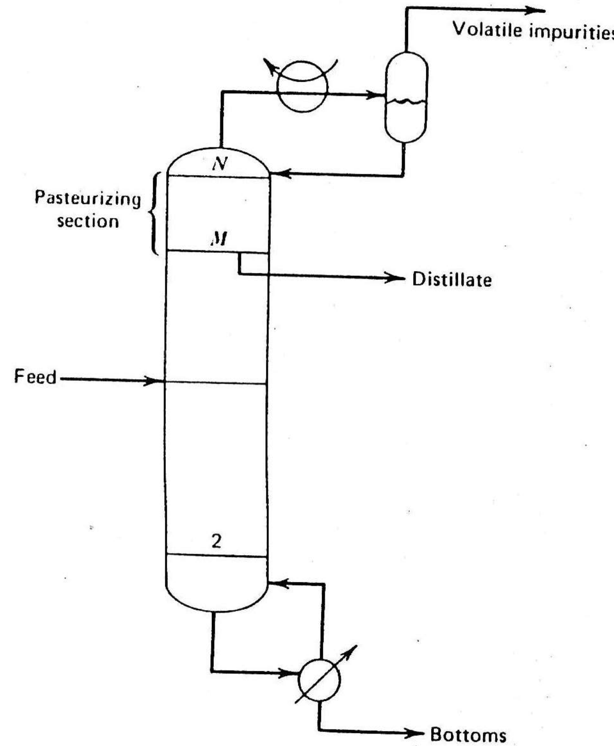
6.19 When the feed to a distillation column contains a small amount of impurities that are much more volatile than the desired distillate, it is possible to separate the volatile impurities from the distillate by removing the distillate as a liquid side stream from a stage located several stages below the top stage. As shown below, this additional top section of stages is referred to as a *pasteurizing section*.
(a) Determine the number of degrees of freedom for the unit.
(b) Determine a reasonable set of design variables.

6.20 A system for separating a mixture into three products is shown below. For it, determine:
(a) The number of variables.
(b) The number of equations relating the variables.
(c) The number of degrees of freedom.
and propose:
(d) A reasonable set of design variables.

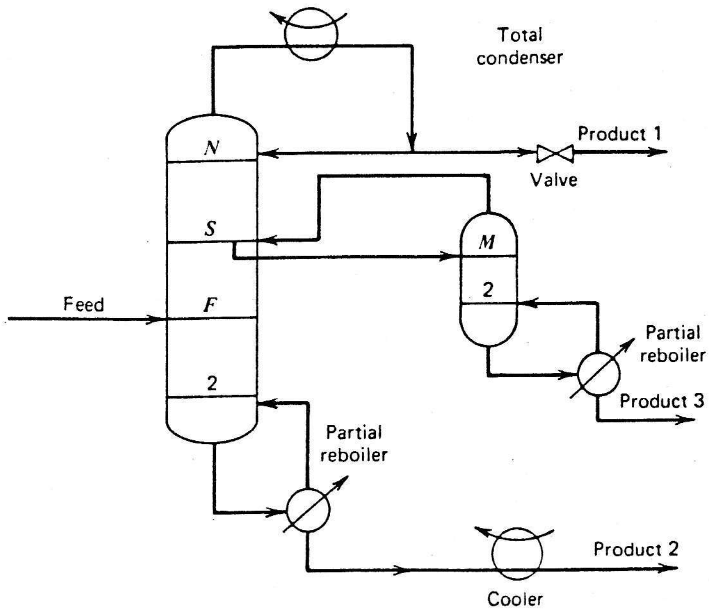
Problem 6.18



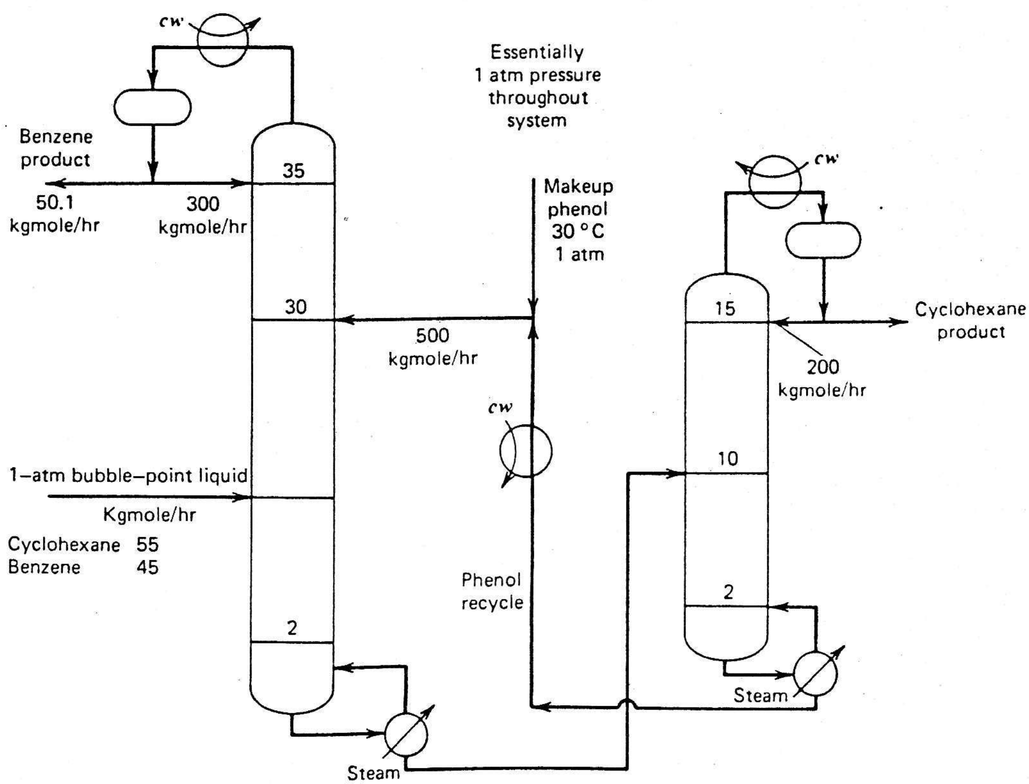
Problem 6.19



Problem 6.20



Problem 6.21



6.21 A system for separating a binary mixture by extractive distillation, followed by ordinary distillation for recovery and recycle of the solvent, is shown on previous page. Are the design variables shown sufficient to completely specify the problem? If not, what additional design variable(s) would you select?

6.22 A single distillation column for separating a three-component mixture into three products is shown below. Are the design variables shown sufficient to specify the problem completely? If not, what additional design variable(s) would you select?