u = velocity of fluid
u_m = maximum fluid velocity in tube
$\bar{u}$ = average fluid velocity in tube
x = axial distance

Greek Letters

α_n = positive roots of $J_1(\alpha) = 0$
β_n = eigenvalues of Equation (8)
Γ = gamma function
η = $1 - \xi$
κ = $k/C\bar{u}\rho$
λ = parameter
μ = viscosity of fluid
ξ = normalized distance variable, $(= r/r_o)$

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Optimum Design of Conventional and Complex Distillation Columns

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A method is proposed for achieving the optimum design, in the sense of minimum plates, for conventional and complex distillation columns for any set of specifications directly dependent on product purity which might be imposed by the designer. The method uses the calculational procedure of Thiele and Geddes, the θ-method of convergence, and sequential-search procedures. Illustrative examples chosen from a large number of design problems solved by this method are presented.

In the past, calculational methods that used successive approximations in the design of distillation columns were generally based on the calculational procedure of Lewis and Matheson (*10, 13*). These methods are essentially applicable only to the design of distillation columns for which the designer has set separation ratios of key components as the design criteria. Also, certain complex columns cannot be designed by these methods even for specifications of this type.

Hanson (*6*) and Holland (*7*) have proposed the indirect use of the calculational procedure of Thiele and Geddes (*15*) for the design of a column by solving problems for columns with various plate configurations until a solution is obtained or estimated that satisfies the design criteria. A new and more direct method is described herein for determining that plate configuration, for conventional or complex columns, which allows the specifications set by the designer, of any type directly dependent on product purity, to be met or exceeded with the minimum integral number of plates.

This new design method employs the procedure of Thiele and Geddes (*15*), the θ-method of convergence (*7, 11*), and multivariable sequential-search techniques (*1, 8, 16*). In this method, a functional expression or objective function is formed from the product specifications which, in a sense, measures the "distance" between the values specified for the products of the column and the values that are obtained for a particular plate configuration. Initially, sequential-search procedures are used to minimize this objective function for assumed temperature, liquid, and vapor-rate profiles in the column. The θ-method of convergence is then used to obtain new profiles in a manner which ensures that as many of the product specifications will be met exactly as can be obtained with an integral number of plates in each section of the column. The sequential-search procedure is continued until a minimum (relative or global) for the objective function is obtained. It should be noted that the proposed method, while not approximate, avoids the necessity of determining the minimum reflux ratio and the minimum total number of plates, quantities which are required by most approximate methods (*2, 3, 4*). For example, in the use of the proposed method in the design of conventional columns, two of the inputs consist of the ranges of the independent variables N and M. If a reflux ratio less than the minimum is specified by the designer, the proposed method gives the solution corresponding to the N and M (most probably N_{max} and M_{max}) for which the objective function is minimized over the range of N and M considered.

DESIGN OF CONVENTIONAL COLUMNS

The following description of the proposed design procedure is divided into three parts: the formulation of the objective function, the initial search, and the final search.

Formulation of the Objective Function

In order to apply modern search techniques to this problem, it is necessary to formulate an objective function that is to be minimized by the proper choice of the independent variables (N,M). Fortunately, the objective function may be stated in terms of the g functions introduced by Lyster et al. (*11*) (see also reference 7). For the design of a conventional column, the objective function takes the following form

$$O(N,M) = \sqrt{g_1^2 + g_2^2} \qquad (1)$$

The g functions or specification functionals g_1 and g_2 are obtained from the specifications set by the designer. As shown below, the g functions constitute a measure of the difference between the calculated and specified values of the selected design variables. Also, the specifications and corresponding g functions that follow are formulated such that the total number of plates tends to a minimum as the g functions tend to zero. Further physical significance may be associated with the objective function as follows. Let g_1 and g_2 be plotted along the vertical and horizontal axes. Thus, each set of values, N and M, gives rise to a point in the g_1g_2 plane, and the distance $(\sqrt{g_1^2 + g_2^2})$ of this point from the origin is seen to be equal to the value of the objective function. Thus, in view of the nature of the g functions, the desired solution (N,M) is seen to be the one that minimized the objective function or the distance $\sqrt{g_1^2 + g_2^2}$. Actually, the objective function could be stated in terms of the sum squares of the g functions or perhaps the sum of the absolute values of the g functions. However, the proposed form was selected over other possible forms because it preserved the distance concept. For three typical sets of design specifications for a conventional column, the specification functionals are as follows:

A. Specifications: L_o/D; $\left(\frac{b_l}{d_l}\right) \leqq \left(\frac{b_l}{d_l}\right)_{spec}$; $\left(\frac{b_h}{d_h}\right) \geqq \left(\frac{b_h}{d_h}\right)_{spec}$

$$\left.\begin{aligned} g_1(N,M) &= (d_l)_{ca} - (d_l)_{spec} \\ g_2(N,M) &= (d_h)_{ca} - (d_h)_{spec} \end{aligned}\right\} \qquad (2)$$

It is to be noted that for any given value of the separa-

TABLE 1. FEED COMPOSITION AND TOWER CONDITIONS FOR EXAMPLE PROBLEMS

Tower pressure: 300 lb./sq. in. abs.; a partial condenser is employed.
Product conditions: Distillate is removed as dew-point vapor. Bottoms and all sidestream products are removed as bubble-point liquids.
Feed conditions: Feeds enter as bubble-point liquids. The feed compositions are as listed below:

Component	Composition 1 Mole fraction	Composition 2 Mole fraction
Methane	0.050	0.020
Ethane	0.100	0.100
Propylene	0.150	0.060
Propane	0.150	0.125
Isobutane	0.150	0.035
n-Butane	0.100	0.150
n-Pentane	0.100	0.152
Hexane	0.100	0.113
Heptane	0.050	0.090
Octane	0.030	0.085
400 normal boiling point	0.020	0.070
	Bubble point 63.018°F.	Bubble point 164.442°F.

Vapor-liquid equilibrium data and enthalpy data are listed in reference 7.

TABLE 2. PRODUCT SPECIFICATIONS FOR EXAMPLE PROBLEMS

Example 1. Conventional column with a feed rate of 100 moles/hr. of composition 2. Design specifications: for a reflux ratio, L_o/D, of 2.0, the separation ratios of the light and heavy key components shall be as follows.

$$\left(\frac{b_l}{d_l}\right) \leqq 0.56699561 \times 10^{-7}$$
$$\left(\frac{b_h}{d_h}\right) \geqq 0.39292070 \times 10^{30}$$

Example 2. Conventional column with a feed rate of 100 moles/hr. of composition 2. Design specifications: for a reflux ratio, L_o/D, of 2.0, the dew point of the distillate $T_{D.P.}$, and the distillate flow rate D shall be as follows.

$$T_{D.P.} \leqq 108°\text{F.}$$
$$D = 31.6 \text{ moles/hr.}$$

(Note: The specifications for the two problems above may be met exactly by a conventional column with seven rectifying plates and seven stripping plates. Thus, $O(7, 7) = 0$ is the global minimum.)

Example 3. Complex column with two feeds and two products. The feeds are $F_1 = 100$ moles/hr. and $F_2 = 100$ moles/hr. of compositions 1 and 2, respectively. Design specifications: for a reflux ratio, L_o/D, of 2.0, the separation ratios of the light and heavy key components shall be as follows.

$$\left(\frac{b_l}{d_l}\right) \leqq 0.61690594 \times 10^{-8}$$
$$\left(\frac{b_h}{d_h}\right) \geqq 0.11480398 \times 10^{24}$$

(Note: These specifications can be met exactly by a column with twenty plates where F_1 is introduced at plate 8 and F_2 is introduced at plate 13. Thus $O(7, 5, 8) = 0$ is the global minimum.)

Example 4. Complex column with one feed and three products. The feed is 100 moles/hr. of composition 2. Design specifications: for a reflux ratio, L_o/D, of 2.0, the dew point of the distillate $T_{D.P.}$; the bubble point of the sidestream, T_{W_1}; the distillate rate D; and the sidestream rate W_1 shall be as follows.

$$T_{D.P.} \leqq 134°\text{F.}$$
$$T_{W_1} \cong 208°\text{F.}$$
$$D \geqq 35 \text{ moles/hr.}$$
$$W_1 \geqq 5 \text{ moles/hr.}$$

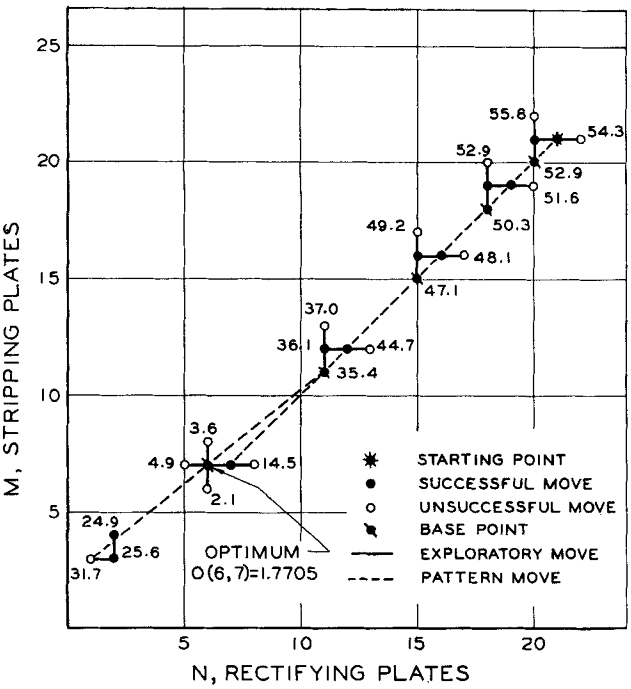

Fig. 1. Initial moves of the pattern search for the design of a conventional column, example 1.

tion ratio b_i/d_i, the corresponding value of d_i is obtained by an overall material balance.

$$(d_i)_{ca} = \frac{FX_i}{1 + \left(\frac{b_i}{d_i}\right)_{ca}} \tag{3}$$

B. Specifications: L_o/D; $T_{D.P.} \leqq (T_{D.P.})_{spec}$; $D = D_{spec}$

$$\left.\begin{aligned} g_1(N,M) &= \sum_{i=1}^{c} \frac{(d_i)_{ca}}{(K_{Di})_{spec}} - \sum_{i=1}^{c} (d_i)_{ca} \\ g_2(N,M) &= \sum_{i=1}^{c} (d_i)_{ca} - D_{spec} \end{aligned}\right\} \tag{4}$$

Instead of the equality $D = D_{spec}$, the inequality $D \geqq D_{spec}$ may be imposed by the designer. However, the total distillate rate may not be as sensitive an index of product purity as separation ratios or the dew-point temperature or bubble-point temperature of the distillate. So generally the specification D_{spec} is met exactly during the final search, as will be discussed in a later section.

C. Specifications: L_o/D; $\left(\frac{b_l}{d_l}\right) = \left(\frac{b_l}{d_l}\right)_{spec}$; $D = D_{spec}$

$$\left.\begin{aligned} g_1(N,M) &= (d_l)_{ca} - (d_l)_{spec} \\ g_2(N,M) &= \sum_{i=1}^{c} (d_i)_{ca} - D_{spec} \end{aligned}\right\} \tag{5}$$

An equivalent set of specifications may be written involving the heavy-key separation ratio. The restrictions on the use of an inequality for the total distillate rate specification instead of the equality $D = D_{spec}$ are the same as those mentioned above.

Initial Search

On the basis of assumed sets $\{T\}$, $\{L\}$, and $\{V\}$, it is desired to determine that pair of values N and M for which $O(N,M)$ is a minimum. Due to the nonlinear form of the equations describing distillation processes, it is not possible to derive an analytical expression for $O(N,M)$ in terms of N and M without making simplifying assumptions about the problem (*12*). Sequential-search methods do not require an analytical expression for the objective function in terms of the independent variables in order to perform the minimization.

Since N and M here must be integral numbers, gradient methods of search, which require numerical approximations of the partial derivatives of the objective function with respect to the independent variables, are not applicable. The authors have had good success with the pattern search of Hooke and Jeeves (*8*) and a multivariable extension of the lattice search of Wilde (*16*). However, because of the lower computation time required with the pattern search for the design of complex columns, only this optimization method will be discussed further.

When each component-material balance encloses only one plate, the resulting set of equations for an entire column may be stated in the form of a tridiagonal matrix. For assumed sets $\{T\}$, $\{L\}$, and $\{V\}$ the component-material balances reduce to a system of linear equations in the v_{ji}'s or l_{ji}'s. These equations may be solved for all of the component flow rates, for each pair of values N and M, by use of a simple algorithm described by Grabbe et al. (*5*) and Lapidus (*9*) for handling tridiagonal matrices. The values of d_i and b_i so obtained are used to evaluate the objective function $O(N,M)$. In the pattern search, small changes in the independent variables (or exploratory moves) are made about the starting point to determine the direction in which larger changes (or pattern moves) should be made. A point located by exploratory moves is termed a base point if at that point the objective function has the lowest value so far obtained. Pattern moves are extrapolated moves through succesive base points, corresponding to a vector from the last base point with components obtained by the changes in the independent variables between the last two base points.

Figure 1 illustrates the moves of the initial pattern search for the design of a conventional distillation column (see Table 1 and example 1 in Table 2). The starting point (21, 21) was chosen for this illustrative example in order to portray the path taken by the pattern search over a wide range of values of the independent variables N and M. For some specification functionals, $O(N,M)$ may be a multimodal function (more than one minimum), and thus in practice the initial search procedure is started near the origin to seek that extreme value of $O(N,M)$ for which $(N + M)$ is smallest.

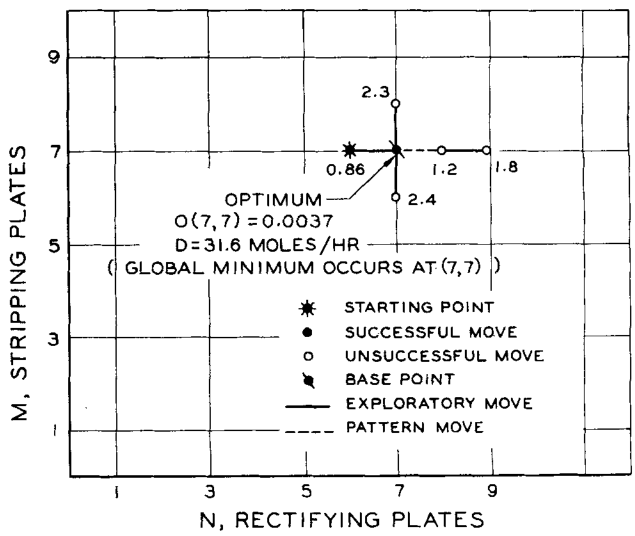

Fig. 2. Final moves of the pattern search for the design of a conventional column, example 1.

As shown in Figure 1, the first exploratory move in a series is an increase along the abscissa. Thus, from the starting point (21, 21), the point (22, 21) was investigated, and no reduction in the value of $O(N,M)$ was obtained. The move to (20, 21) was successful so (20, 22) was tried next. This failed; (20, 20) was tried, with success. The point (20, 20) became a base point, and a pattern move was made to (19, 19). It will be noted that the pattern moves become longer as a successful trend is established. If the exploratory moves fail to locate a new base point, the search returns to the last base point, and exploratory moves are completed about it. If, for the smallest change allowable in the independent variables, here one plate, the exploratory moves do not reduce the value of the objective function, the search is terminated.

For problems where separation ratios have been specified, some exploratory moves may result in the same value of the objective function to eight significant digits, which results from a "pinch condition" (7) in the column caused by the use of too many plates. This difficulty was overcome by causing the search procedure to accept that plate configuration having the lowest number of plates when equal values of the objective function were obtained. In addition, for problems with specifications of this type, it was found convenient to use a logarithmic form of the objective function because of the great difference in magnitudes between separation ratios.

$$O(N, M) = \sqrt{\left[\log_e \frac{(b_l/d_l)_{spec}}{(b_l/d_l)_{ca}}\right]^2 + \left[\log_e \frac{(b_h/d_h)_{spec}}{(b_h/d_h)_{ca}}\right]^2} \tag{6}$$

It should be noted that the material-balance equations need be solved only for the key components during the initial search when separation ratios are specified.

Final Search

The final search procedure is started at the final point located by the initial search procedure. In the final search, the sets $\{T\}$, $\{L\}$, and $\{V\}$ are adjusted by use of the θ-method of convergence (7, 11) in conjunction with the computational procedure of Thiele and Geddes (15). New temperature profiles are determined by the K_b-method (7), which eliminates the need for iterative bubble-point calculations, and new sets $\{L\}$ and $\{V\}$ are computed by enthalpy balances by the constant-composition and Q-methods (7).

For conventional columns, the θ-method of convergence can be used to drive either g_1 or g_2 to zero; that is, the sets $\{T\}$, $\{L\}$, and $\{V\}$ will be adjusted so that one or the other of the product specifications will be satisfied exactly. Then the objective function reduces essentially to the absolute value of the other specification functional. For each pair of values N and M considered in the final search, three to five trials of the θ-method of convergence are performed to drive θ approximately to one and the desired specification functional approximately to zero. The equations for the θ-method of convergence and the corresponding objective function $O(N,M)$ for the three typical types of specifications [A, B, C, or Equations (2) through (5)] for a conventional column are given below. In these expressions, the quantity $(d_i)_{co}$ is defined by

$$(d_i)_{co} = \frac{FX_i}{1 + \theta\left(\frac{b_i}{d_i}\right)_{ca}} \tag{7}$$

A. (1) $g_1 = 0$; $O(N,M) = |g_2|$

$$\left.\begin{aligned} g_1(\theta) &= (d_l)_{co} - (d_l)_{spec} \\ D &= \sum_{i=1}^{c} (d_i)_{co} \\ g_2(N,M) &= (d_h)_{co} - (d_h)_{spec} \end{aligned}\right\} \tag{8}$$

In this case, the θ-method is used to make $g_1(\theta) = 0$ for each choice of N and M. Note that θ is found directly by setting $g_1(\theta) = 0$ and by solving for θ. Then as implied by Equation (8), D is calculated by use of Equation (7) for each component. After sets $\{T\}$, $\{L\}$, and $\{V\}$ have been found such that $g_1(1) \cong 0$, the value of $O(N,M)$ is computed by use of the expression given above for g_2. This process is repeated for different sets of N and M selected by the search technique until a set is found for which $O(N,M)$ or $|g_2|$ is a minimum. The remaining cases are handled in an analogous manner.

A. (2) $g_2 = 0$; $O(N,M) = |g_1|$

$$\left.\begin{aligned} g_2(\theta) &= (d_h)_{co} - (d_h)_{spec} \\ D &= \sum_{i=1}^{c} (d_i)_{co} \\ g_1(N,M) &= (d_l)_{co} - (d_l)_{spec} \end{aligned}\right\} \tag{9}$$

B. (1) $g_1 = 0$; $O(N,M) = |g_2|$

$$\left.\begin{aligned} g_1(\theta) &= \sum_{i=1}^{c} \frac{(d_i)_{co}}{(K_{Di})_{spec}} - \sum_{i=1}^{c} (d_i)_{co} \\ D &= \sum_{i=1}^{c} (d_i)_{co} \\ g_2(N,M) &= \sum_{i=1}^{c} (d_i)_{co} - D_{spec} \end{aligned}\right\} \tag{10}$$

B. (2) $g_2 = 0$; $O(N,M) = |g_1|$

$$\left.\begin{aligned} g_2(\theta) &= \sum_{i=1}^{c} (d_i)_{co} - D_{spec} \\ g_1(N,M) &= \sum_{i=1}^{c} \frac{(d_i)_{co}}{(K_{Di})_{spec}} - \sum_{i=1}^{c} (d_i)_{co} \end{aligned}\right\} \tag{11}$$

C. (1) $g_1 = 0$; $O(N,M) = |g_2|$

$$\left.\begin{aligned} g_1(\theta) &= (d_l)_{co} - (d_l)_{spec} \\ D &= \sum_{i=1}^{c} (d_i)_{co} \\ g_2(N,M) &= \sum_{i=1}^{c} (d_i)_{co} - D_{spec} \end{aligned}\right\} \tag{12}$$

C. (2) $g_2 = 0$; $O(N,M) = |g_1|$

$$\left.\begin{aligned} g_2(\theta) &= \sum_{i=1}^{c} (d_i)_{co} - D_{spec} \\ g_1(N,M) &= (d_l)_{co} - (d_l)_{spec} \end{aligned}\right\} \tag{13}$$

Cases B(1) and C(1) would result from specifications for the distillate rate involving inequalities. As before, D may not be as sensitive an index of product purity as other quantities, such as separation ratios. Also, since D is a quantity that can be set with a good deal of logic by the designer, and since specifications involving D are very quickly met with the θ-method of convergence, the investigation of the proposed design method generally concerned itself with exact satisfaction of the distillate rate specification whenever it was specified.

If the product specifications set by the designer can be met exactly by a column with an integral number of plates in each section, and if this column is the solution for which $(N + M)$ is minimum, then only one solution will be obtained regardless of which of the two specification functionals is driven to zero by the θ-method of convergence. If the product specifications cannot be met exactly with an integral number of plates, two solutions will be obtained. In many cases, the final plate configuration remains the same for the two solutions, while the distillate rates and sets $\{T\}$, $\{L\}$, and $\{V\}$ differ. In other cases the plate configurations differ as well.

To demonstrate another characteristic of the objective function, consider Equations (2) and (9). Note that the final search seeks the set (N,M) such that b_1/d_1 is closest to the specified value; that is, it seeks to minimize $|g_1|$. Thus, the final search does not distinguish between values of g_1 of the same magnitude but of different sign; whereas, in the original specification [specification A, Equation (2)], a positive value of g_1 is to be preferred over a negative value of the same magnitude. However, the pattern search terminates only when points (N,M) on all four sides of the final point yield higher values of the objective function. Thus, if at the final point (N,M) where $|g_1|$ is a minimum $g_1 < 0$, two of the four neighboring points, one along each coordinate axis, constitute solutions for which $g_1 > 0$.

Figure 2 illustrates the final search for example 1, Table 2. The starting point (6, 7) is the final point located by the initial search. For this problem, the θ-method of convergence was used to make $g_2 = 0$, and the pattern search was used to minimize $|g_1|$ [see Equation (9)]. In this case the minimum value of $|g_1|$ found was zero; consequently, the specifications could be met exactly by use of an integral number of plates (7, 7) in each section of the column. A complete description of this solution is presented in tabular form elsewhere.* Essential information regarding the solutions of the other examples in Table 2 is presented either in Figure 3 or in tabular form* or in both sources. Complete descriptions of the solutions of these and other design problems are given in reference *14*.

* Tabular material has been deposited as document 8372 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for 1.25 for photoprints or 1.25 for 35 mm. microfilm.

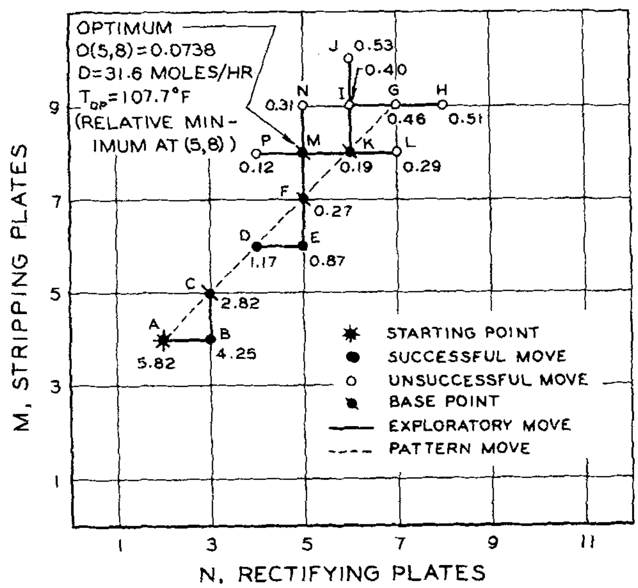

Fig. 3. Final moves of the pattern search for the design of a conventional column, example 2.

It will be noted that the starting point of the final search in example 1 was only one plate away from the solution finally obtained. For a large number of design problems involving hydrocarbon feeds and complex columns, it has been found that for problems with specifications involving only separation ratios the final point located by the initial search is very close to the solution obtained in the final search, despite fairly large differences in the sets $\{T\}$, $\{L\}$, and $\{V\}$ initially assumed.

Because of this observation, it is felt that the final point located by the initial search would be a good estimate of the optimal solution for design problems involving only separation ratios. Since only the material-balance equations for the key components need be solved during the initial search, such an estimate is more easily and quickly obtained than those estimates based on conventional short-cut methods. This relative independence of the profiles assumed initially has not been found to be the case for problems involving other specifications, as will be discussed in the following section.

MULTIMODAL OBJECTIVE FUNCTIONS

If a plate configuration exists that allows all the product specifications to be met exactly, the objective function will have a value of zero at that point. This will be the pair of values N and M for which $O(N,M)$ is a global minimum. However, this solution to the design problem may not be the optimal solution, since $(N + M)$ may not be a minimum at this point.

Figure 3 presents the final pattern search for example 2, Table 2; the moves proceed alphabetically. It will be seen that the solution obtained for this problem was found at (5, 8) with $D = 31.6$ moles/hr. and $T_{D.P.} = 107.7$°F. During the final search, the specification functional g_2 was driven to zero by use of the θ-method of convergence, and $|g_1|$ was minimized by the pattern search. Since the specification could have been met exactly at (7, 7), it is seen that for the solution at (5, 8) the objective function is a relative minimum. Thus, the optimal solution, here (5, 8), need not occur at the global minimum of the objective function.

Search procedures have no means of distinguishing between minima. Fortunately, the optimal solution is associated with that point at which the objective function takes on an extreme value that is located closest to the origin, since $(N + M)$ will be a minimum there. For this reason, the initial search is started close to the origin. However, for problems where the dew-point temperature of the distillate and the total distillate rate are specified, it has been noted that the effect of the sets $\{T\}$, $\{L\}$, and $\{V\}$ assumed during the initial search on the point located at the end of the initial search is considerably greater than for problems where separation ratios are specified.

Conceivably, the sets $\{T\}$, $\{L\}$, and $\{V\}$ initially assumed for problems of this type could be such that the point located at the end of the initial search would cause the final search to miss the solution closest to the origin and to pick a less desirable solution. To avoid this for problems of this type it has been found convenient to drop the initial search, starting the final search arbitrarily near the origin. Alternatively, the checking procedure described below may be used.

Once the apparent optimal solution has been located by the final search, a check can be made, if desired, to see if a more desirable solution can be obtained. Figure 4 illustrates a way to do this. Any solution to the right of the line (for complex columns this becomes a plane or

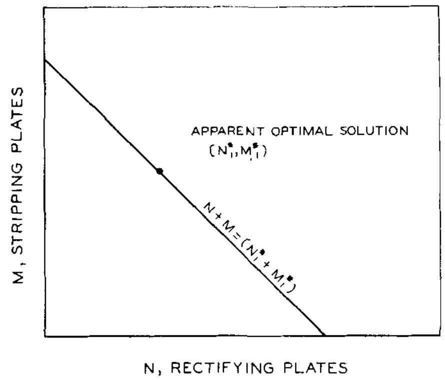

Fig. 4. Procedure for ensuring that the optimal solution is located by final searching procedure.

hyperplane) is a less desirable solution, while any point to the left is a more desirable solution. Thus, to see if a more desirable solution exists, the final search may be started again at some new point in the left-hand region. It should be pointed out that for the problems so far solved by the proposed design method, the solutions obtained by the first application of the final search have not been improved upon by restarting the final search from a new point. Also for those problems where the product specifications could be met exactly by a column with a known plate configuration, the solution obtained by the first application of the final search was in each case as good or better, in the sense of minimum plates, than the known plate configuration.

DESIGN OF COMPLEX COLUMNS

The objective function for the design of complex columns is of the same general form as that for conventional columns. The form of the objective function for three types of complex columns will be illustrated.

1. Complex Column with Two Feeds, F_1 and F_2, and Two Products, D and B

For this column, the objective function remains the same as that for a conventional column, except that it now becomes a function of one additional variable.

$$O(N,k_1,M) = \sqrt{g_1^2 + g_2^2} \tag{14}$$

The additional independent variable k_1 refers here to the number of plates between the two feed plates. During the initial and final search, k_1 may take on negative values, indicating a switch in the relative position of the two feed plates. Solutions have been encountered where a switch in the relative position of the two feeds was indicated. Additional feed plates only increase the number of independent variables that must be searched.

2. Complex Column with One Feed, F_1, and Three Products, D, W_1, and B

The number of independent variables is increased by one over that for a conventional column, and the number of specification functionals is increased by two for the sidestream specifications.

$$O(N,k_1,M) = \sqrt{g_1^2 + g_2^2 + g_3^2 + g_4^2} \tag{15}$$

Here k_1 refers to the number of plates between the sidestream plate and the feed plate, and once again k_1 may take on negative values, indicating a switch in the relative position of the feed plate and sidestream plate.

3. Complex Column with Two Feeds, F_1 and F_2, and Four Products, D, W_1, W_2, and B

There are five independent variables for this problem and six specification functionals in the objective function, two for each sidestream and the distillate.

$$O(N,k_1,k_2,k_3,M) = \sqrt{g_1^2 + g_2^2 + g_3^2 + g_4^2 + g_5^2 + g_6^2} \tag{16}$$

SEARCHING PROCEDURE

The initial search remains the same as that for conventional columns. In the final search, one-half of the specification functionals, one for each sidestream and the distillate, are driven to zero by the θ-method of convergence for complex columns (*7, 11*). The results of the final pattern search for the design of a complex column with two feeds and two products (example 3, Table 2) are shown elsewhere.* The initial search terminated at (6, 1, 9), the starting point for the final search as well as the final solution. The final solution (6, 1, 9) is a relative minimum, and four fewer plates were needed to satisfy the specifications here than at the global minimum (*7*; 5, 8).

In using the pattern search for the design of complex columns, the exploratory and pattern moves are made in the same general way as that described for conventional columns. The pattern moves are again extrapolated moves between successive base points. For example, for a complex column with one feed and one sidestream, suppose the nth base point is $P_n\ [N_n,k_{1,n},M_n]$ and the next base point is $P_{n+1}\ [N_{n+1},k_{1,n+1},M_{n+1}]$; then the pattern move will be to the point P, namely

$$P\,[N_{n+1} + (N_{n+1} - N_n),\ k_{1,n+1} + (k_{1,n+1} - k_{1,n}),\ M_{n+1} + (M_{n+1} - M_n)]$$

The extension to a complex column with any number of independent variables is obvious.

Example 4 of Table 2 was used to illustrate the application of the search method for the design of a complex column with one feed and three products (one sidestream). The moves of the final pattern search for this problem are presented elsewhere.* The specified values of the dew-point temperature of the distillate $T_{D.P.}$ (represented by the functional g_1), and the flow rate W_1 of the sidestream (represented by the functional g_3) were met exactly, $g_1 = g_3 = 0$, by the θ-method of convergence, where

$$\left.\begin{aligned} g_1(\theta_1,\theta_2) &= \sum_{i=1}^{c} \frac{(d_i)_{co}}{(K_{Di})_{spec}} - \sum_{i=1}^{c} (d_i)_{co} \\ g_3(\theta_1,\theta_2) &= \sum_{i=1}^{c} (w_{1i})_{co} - (W_1)_{spec} \end{aligned}\right\} \tag{17}$$

and where

$$(d_i)_{co} = \frac{FX_i}{1 + \theta_1\left(\dfrac{b_i}{d_i}\right)_{ca} + \theta_2\left(\dfrac{w_{1i}}{d_i}\right)_{ca}}$$

$$(w_{1i})_{co} = \theta_2\left(\frac{w_{1i}}{d_i}\right)_{ca}(d_i)_{co}$$

The two remaining specifications, D and T_{w_1}, were represented by the specification functionals g_2 and g_4, respectively. The objective function to be minimized by the final search was

$$O(N,k_1,M) = \sqrt{g_2^2 + g_4^2} \tag{18}$$

where

$$g_2(N,k_1,M) = \sum_{i=1}^{c} (d_i)_{co} - D_{spec}$$

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* See footnote on p. 699.

$$g_4(N,k_1,M) = \sum_{i=1}^{c} (w_{1i})_{co} K_i \Big|_{T_{w_1}} - \sum_{i=1}^{c} (w_{1i})_{co}$$

Of these two specifications, the more important for this problem was D, which was set as an inequality. The final search was biased toward satisfaction of this specification. This point will be discussed in more detail below.

The objective function during the final search consists of only one-half of the specification functionals for the problem. Thus, for complex columns with sidestreams, it is evident that two or more specification functionals remain in the objective function during the final search. Minimization of the objective function again minimizes the distance of the specification functionals (that is, the square root of the sum of their squares) from an origin (a point where the g functionals of O have the value of zero). For problems where all of the specifications are set as inequalities, it is possible that one or more of the specifications remaining to be satisfied after use of the convergence method, while close to being met exactly, will still be unsatisfied in the sense of the inequality. This is because the objective function depends upon the absolute values of selected g functionals, because with the integral number of plates used, the product specifications cannot be met exactly. For conventional columns and for complex columns with several feeds but no sidestreams, if an inequality remains unsatisfied at the final minimum, two points or more adjacent to the final minimum will always satisfy this inequality. This assurance cannot be given when the objective function in the final search contains more than one nonzero specification functional.

If it is imperative that the inequalities corresponding to the remaining nonzero specification functionals be satisfied, in addition to those satisfied by the convergence method, the final search procedure can be reset to search a solution with more plates. Alternatively, if only one of the remaining inequalities is critical, weighting factors may be used to bias the final search as desired. For example, the objective function given by Equation (18) may be reformulated as follows:

$$O(N,k_1,M) = \sqrt{a_2 g_2^2 + a_4 g_4^2} \quad (19)$$

where a_2 and a_4 are positive constants that may be selected as desired to produce bias in the final search.

Although considerable discussion has been devoted to the fine points associated with the statement of the specifications in terms of inequalities, it is anticipated that the solution associated with the first minimum of the objective function found by the final search will be satisfactory for most design problems.

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NOTATION

- b_i = molal withdrawal rate of component i in the bottom product from the column
- c = total number of components
- F_1, F_2 = molal rate for feed stream 1 or 2
- FX_i = total molal rate of component i entering the column in the feed
- d_i = molal withdrawal rate of component i in the distillate from the column
- D = total molal withdrawal rate of the distillate
- g = specification functional expression
- K_{Di} = equilibrium constant for component i at the temperature of the distillate
- K_{ji} = equilibrium constant for component i at the temperature of plate j
- k = number of plates between sidestream plate and feed plate or between two feed plates
- L = molal flow rate of liquid leaving a plate
- L_o = molal reflux rate
- l_{ji} = molal flow rate of component i in the liquid leaving plate j
- M = number of plates below the lowest feed plate or sidestream plate, including that plate
- N = number of plates above the uppermost feed plate or sidestream plate
- O = objective function, defined by equations in the text
- T = plate temperature
- $T_{D.P.}$ = dew point temperature of the distillate
- T_{wj} = bubble point temperature of sidestream j
- V = molal flow rate of vapor leaving a plate
- v_{ji} = molal flow rate of component i in the vapor leaving plate j
- w_{ji} = molal withdrawal rate of component i in sidestream j
- W_j = total molal withdrawal rate of sidestream j

Subscripts, Superscripts, and Symbols

- $*$ = optimal value found for a given set of conditions
- θ_1, θ_2 = multipliers, see references *7* and *11*
- $\{\ \}$ = set of values, here one for each plate in the column
- h = heavy key component
- l = light key component
- ca = calculated value
- co = value corrected by θ-method of convergence, see references 7 and *11*
- $spec$ = specified value
- $A|B$ = quantity A evaluated at the condition B

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