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# A Calculational Procedure for Design Problems in Multicomponent Distillation

**A calculation procedure for multicomponent distillation has been developed that is directly applicable to design problems. It is based on successive approximation methods with adjustment of the number of equilibrium stages in each column section between iterations to meet given reflux flow and feed stage composition conditions while maintaining specified key component recoveries. This procedure has been applied to a number of representative distillation design problems. It converges readily to proper column designs from initial estimates based on a noniterative stage-to-stage calculation. Moreover, the procedure is markedly superior in computational efficiency to solution of design problems by repeated application of operating calculations to assumed column configurations.**

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## SCOPE

Calculational problems in multicomponent distillation can be divided into two general types: (1) operating problems where the separation that can be obtained with a given column configuration under given conditions is to be found; and (2) design problems where the column configuration and operation to meet desired separation specifications is to be determined.

Quite different approaches are necessary for the solution of these two classes of problems. For the operating problem approximate solutions can be obtained by group methods such as those of Underwood (1946, 1948). When more exact calculations are required the widely used successive approximation methods can be employed, either as a modification of the classical procedure of Thiele and Geddes (1933) or the more recent, and highly effective, matrix approaches as by Napthali and Sandholm (1971).

For the design problem the situation is not so well in hand. Approximate solutions can be derived from calculations of minimum stages (Underwood, 1932; Fenske, 1932) and minimum reflux (Underwood, 1946, 1948), together with an empirical correlation of required stages and reflux (Gilliland, 1940; Erbar and Maddox, 1961). Group methods can also be used. However, where more exact calculations are necessary no really satisfactory techniques have been available. Stage-to-stage methods (Lewis and Matheson, 1932; Waterman and Frazier, 1965) have severe convergence difficulties for many distillation cases and have not found general acceptance. The successive approximation methods are, unfortunately, not directly applicable, since they are dependent on the number of stages being specified. Very frequently, however, these methods are employed in the solution of design problems by their application to several related operating problems with different numbers of stages. This is repeated until a solution is found that satisfies the design separation requirements. Although this shotgun approach often is successful, it can be a very inefficient and tedious process. There has long existed the need for calculational methods specifically suited to the design of multicomponent distillation columns and capable of results of an accuracy equivalent to those of the better operating calculations.

The aim of this study has been the development of such a computer-oriented design procedure for simple multicomponent distillation columns, that is, for columns with a single feed and only two products. The design specifications are taken to include key component recoveries, optimum feed location, and a set economic multiple of minimum reflux ratio. This work has been based upon the successive approximation matrix methods and the concept of adjustment of numbers of stages above and below the feed between iterations to satisfy design specifications. Moreover, a procedure has been sought that can provide detailed solutions to a design problem at computational expense comparable to that required for equivalent solutions to operating problems rather than at several times operating solution costs as required by shotgun techniques.

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## CONCLUSIONS AND SIGNIFICANCE

The design successive approximation (DSA) procedure formulated in this work operates by incorporating key component recovery specifications in the equation set used at each successive approximation iteration and allowing reflux rates to be a dependent variable in these equations. The estimates that the iteration yields for column variables (compositions, flows, temperatures) both constitute the base values for the next iteration and are utilized as the source of information for correction of column configuration. The procedure operates in a manner similar to a matrix type successive approximation operating calculation, but with numbers of stages changing between iterations and converging to the required numbers of stages more or less simultaneously with convergence of the column variables.

This DSA procedure has been found to be very effective in the solution of representative design problems in multicomponent distillation (Ricker, 1972). The method retains the flexibility and precision of the well-established matrix methods for operating problems (Naphtali and Sandholm, 1971). At the same time it usually obtains solutions to a design problem for a calculational effort equivalent to less than two operating problem calculations. If operating calculations are applied to a design problem with a shotgun approach, far more than two such calculations are generally required. In addition to providing significantly improved computational efficiency, the DSA procedure eliminates the necessity for formulation and revision of a number of operating problems in the course of a multicomponent distillation design.

Although the DSA procedure has been implemented for only one type of design problem specifications, that is, key component recoveries and a given multiple of minimum reflux, application of the method to other combinations of specifications requires only relatively minor changes in details of implementation. Thus the method should be an effective tool for design calculations for many types of simple distillation columns commonly encountered in the chemical industry.

### MULTICOMPONENT DISTILLATION

The well-known equations describing continuous multicomponent distillation derive from the requirements for conservation of material and heat, and for phase equilibrium, on each theoretical stage (for example, King, 1971). Figure 1 depicts a general stage $j$ in a column of $N$ stages, numbered upward from the (equilibrium) reboiler. At fixed pressure and in the absence of external heat transfer, the condition on each stage is described in terms of the temperature $T_j$, the liquid and vapor flows $L_j$ and $V_j$, and the component mole fractions $x_{ij}$ and $y_{ij}$ for the $M$ components present. For an equilibrium condition represented by

$$y_{ij} = K_{ij}x_{ij}$$

the variables for any stage are related by component material balances

$$V_{j-1}y_{i,j-1} - (L_j + K_{ij}V_j)x_{ij} + L_{j+1}x_{i,j+1} = (-f_{ij}) \tag{1}$$

where the feed rates $f_{ij}$ occur only on the feed stage. These component balances sum to the overall material balance

$$V_{j-1} - (L_j + V_j) + L_{j+1} = (-F_j) \tag{2}$$

There is also the enthalpy balance requirement

$$V_{j-1}\sum_{i=1}^{M} K_{i,j-1}x_{i,j-1}H_{i,j-1} - \sum_{i=1}^{M}(L_jh_{ij} + V_jK_{ij}H_{ij})x_{ij} + L_{j+1}\sum_{i=1}^{M} h_{i,j+1}x_{i,j+1} = 0 \tag{3}$$

with an additional term appearing on the right-hand side for the feed stage. Finally there is the requirement that vapor and liquid mole fractions sum to unity, which can be expressed

$$\sum_{i=1}^{M}(1 - K_{ij})x_{ij} = 0\,. \tag{4}$$

The column is thus described by $N(M + 3)$ equations. Since the equations are nonlinear and cannot be decoupled, iterative approaches to their solution are required.

In the successive approximation methods which are usually used in detailed distillation calculations, the distillation equations are grouped by type. Values of required unspecified variables are estimated and corrected iteratively until the equation set is satisfied. The classical procedure of this type is that of Thiele and Geddes (1933); many modifications and improvements of this procedure have been developed (for example, Lyster et al., 1959; Hansen et al., 1962; Newman, 1963; Tomich, 1970; Seppala and Luus, 1972). Each has advantages in the solution of operating problems, but for most problems the later simultaneous correction (SC) procedures of Naphtali and Sandholm (1971) and Goldstein and

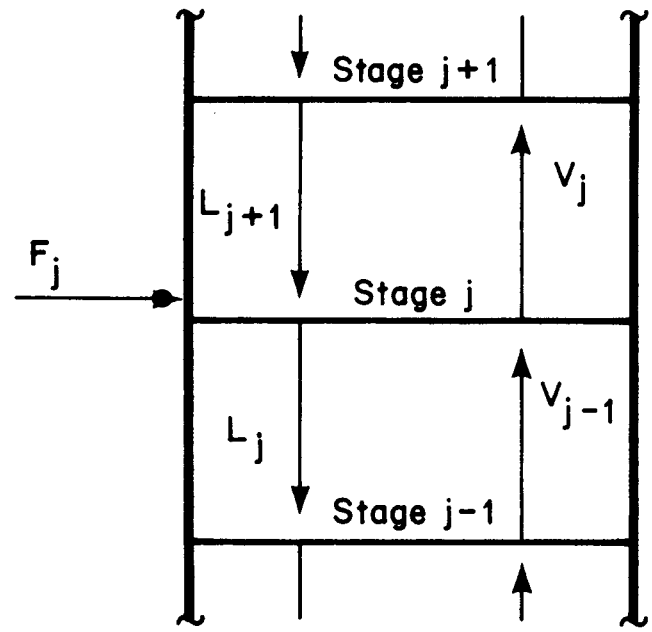


Fig. 1. Representation of a theoretical stage.

Stanfield (1970) seem clearly advantageous. These treat all system equations simultaneously by a multidimensional Newton-Raphson iteration to obtain revised estimates of stage compositions, flows, and temperatures. This SC approach is directly applicable to a wide variety of problem specifications, and its rate of convergence is high, given adequate initial estimates of the iteration variables. All of the successive approximation methods, of course, require a fixed number of stages and feed location and are thus applicable only to operating problems. However, the SC type of procedure has the flexibility in specification and implementation necessary to form the basis of a design calculation procedure.

## DESIGN PROBLEM DESCRIPTION

Design specifications for a simple multicomponent distillation in essence fix the separation to be achieved between the key components. In addition to full description of the feed stream and establishment of column pressure, four more specifications are required for a simple column. In principle these may be drawn from a number of possibilities involving separations, feed location, economic reflux, and so forth. The DSA procedure has been developed for one set of specifications considered representative of many design problems without restriction of its application from other combinations of specifications.

Two proper objectives for most distillation designs are the economic optimization of reflux and of feed stage location. However, such optimizations are rarely undertaken since they entail excessive computational effort. Instead, convenient criteria are usually employed that are considered to lead to near optimum design. In this work we have used the common practice of specification of the operating reflux as some set multiple of minimum reflux and the feed stage location as the stage on which the ratio of the key components in the liquid best matches that in the liquid portion of the feed.

The other two specifications indicate the desired separation; they are usually either the purity or the recovery of a key component in a product stream. Here, specification of the recoveries of the light key component in the distillate and the heavy key component in the bottoms are used.

## DESIGN SUCCESSIVE APPROXIMATION PROCEDURE

The DSA procedure is essentially the simultaneous correction (SC) type solution of an operating problem in which the column configuration is adjusted between SC iterations until a configuration (number of stages and feed location) is reached that satisfies the design specifications.

For efficiency of such an approach, two requirements must be satisfied. First, the number of column configurations examined must be kept small. This requires a systematic method for the selection of the next column configuration based on results of previous calculations. Second, the instances where more than one SC iteration is necessary for a given configuration (a column calculation) must be minimized. This means that accurate estimates of compositions, flows, and temperatures must be provided to start a column calculation making the best use of values calculated for previous column configurations.

Each complete iteration of the DSA procedure consists of three successive steps. First, the column configuration of the previous complete iteration is corrected. Then values for the temperatures, flows, and compositions on each stage of the new configuration are estimated. Last, a column calculation is performed for the new column configuration.

### Column Calculations

The column calculation is a very loosely converged solution to an operating problem. Since the column configuration currently being considered sets the number of stages in each column section, only two design specifications can be included in the definition of this problem. The remaining two must be satisfied by subsequent adjustments in column configuration. The feed stage specification, by its nature, is best met by such adjustments. The column calculations could thus incorporate either two recovery specifications or one recovery and the desired reflux. The former approach has been found to have major advantages in convergence behavior (Ricker, 1972). Thus configuration adjustments are made to satisfy feed stage and reflux specifications while the recovery specifications are included in the basic distillation equation system as

$$x_{l,N}D = (/_l)_D \equiv \text{overhead recovery of light key component} \quad (5)$$

$$x_{h,1}B = (/_h)_B \equiv \text{bottoms recovery of heavy key component.} \quad (6)$$

With these modifications an iteration of the column calculation essentially follows the SC procedure described by Naphtali and Sandholm (1971) for operating problems. Convergence criteria for the column calculation must be stringent enough so that the SC results are sufficiently accurate for adjustment of configuration and yet relaxed enough to prevent unnecessary iterations; very satisfactory criteria have been found to be

$$\left| \sum_{i=1}^{M} y_{i,j} - 1 \right| < 0.05 \qquad j = 1, N,$$

coupled with the requirement that the difference between specified and calculated recoveries be quite small, about 2% or less.

### Adjustment of Column Configuration

The incorporation of the two recovery requirements in the column calculations allows a substantial decoupling of effects in the adjustment process for column configuration. This occurs because the location of the optimum feed stage, as a ratio to total stages, is controlled primarily by the desired product compositions. Also, for constant product compositions, the reflux is influenced primarily by the total number of stages, with a change in the feed location having only minor effect (unless the feed is very far from the optimum point). Therefore, the DSA procedure adjusts the total column stages $N$ to satisfy the recovery specification and corrects the ratio of stages in the rectifying section to stages in the stripping section $N_r/N_s$ to satisfy the optimum feed location criterion. These corrections generally exhibit a low degree of interaction, allowing the procedure to converge rapidly.

The adjustment of total stages makes use of the Erbar-Maddox (1961) correlation to linearize the relationship between $N$ and the reflux $R$. The deviation, or error, parameter for total stages based on complete iteration $r$ is defined as

$$E_1^{(r)} \equiv \frac{[N]_e}{[N]_c^{(r)}} - 1 \quad (7)$$

where $[N]_e$ is the stage requirement estimated from the Erbar-Maddox correlation for the desired reflux, and

$[N]_c^{(r)}$ is that for the value of the reflux calculated in the last column calculation. $E_1^{(r)}$ approaches zero when the design specifications are satisfied; it is negative if $N^{(r)}$ is too high and positive if $N^{(r)}$ is too low. This deviation parameter serves as the basis for application of a one-dimensional secant method correction to $N$. This uses only trends in $E_1^{(r)}$ as a function of $N^{(r)}$ and is thus not dependent on the accuracy of the Erbar-Maddox relationship for success.

$$N^{(r+1)} = N^{(r)} - E_1^{(r)} \Big/ \left\{ \frac{E_1^{(r)} - E_1^{(r-1)}}{N^{(r)} - N^{(r-1)}} \right\} \quad (8)$$

For the first correction another method is used, based on a direct scaling from Erbar-Maddox predictions damped to prevent over correction

$$N^{(2)} = N^{(1)} \left(1 + E_1^{(1)}/2\right) \quad (9)$$

All subsequent adjustments utilize Equation (8). However, it is sometimes necessary to limit adjustments that would be very large or to adjust one stage in the correct direction when moves in the wrong direction are predicted (the correct direction is always given by the sign of $E_1^{(r)}$).

Adjustments to the feed stage location, that is, to $N_r/N_s$, are based on the total reflux expressions of Fenske (1932) applied for the stages in each column section

$$N_r = \frac{\ln \left\{ \left(\frac{x_l}{x_h}\right)_D \Big/ \left(\frac{x_l}{x_h}\right)_f \right\}}{\ln \alpha_{lh}} \quad (10)$$

$$N_s = \frac{\ln \left\{ \left(\frac{x_l}{x_h}\right)_f \Big/ \left(\frac{x_l}{x_h}\right)_B \right\}}{\ln \alpha_{lh}} \quad (11)$$

For constant relative volatilities Equations (10) and (11) yield

$$\ln \left(\frac{x_l}{x_h}\right)_f = \frac{\left\{ \ln \left(\frac{x_l}{x_h}\right)_D + \frac{N_r}{N_s} \ln \left(\frac{x_l}{x_h}\right)_B \right\}}{\frac{N_r}{N_s} + 1} \simeq \frac{\text{constant}}{\frac{N_r}{N_s} + 1} \quad (12)$$

The desired feed stage ratio $(x_l/x_h)_F$ and that calculated for the last column configuration $(x_l/x_h)_f^{(r)}$ are used to define the deviation of error parameter for feed location

$$E_2^{(r)} \equiv \ln \left(\frac{x_l}{x_h}\right)_F - \ln \left(\frac{x_l}{x_h}\right)_f^{(r)} \quad (13)$$

The sign of this parameter indicates the proper direction for adjustment of $N_r/N_s$. Because of the behavior indicated by Equation (12), a one-dimensional secant method applied to the parameter $\gamma \equiv 1/(N_r/N_s + 1)$ leads to convergent adjustments to $N_r/N_s$. For the second column configuration, where this method cannot be applied, the results of the calculation of the initial column configuration are searched for the stage in the column where $(x_l/x_h)$ most closely approaches $(x_l/x_h)_F$. The ratio of stages above and below this stage is used as $(N_r/N_s)^{(2)}$. Adjustments in feed location are limited to a change of one third of the distance to the end of the column being approached, and adjustments indicated in the wrong direction are replaced by adjustments of one stage in the correct direction.

#### Estimation of Compositions, Flows, and Temperatures

To start the calculations for new column configuration, estimates for the compositions, flows, and temperatures on its stages must be provided. These are based on the values calculated for the previous column configuration.

The temperatures are estimated on the basis of the general similarity of column temperature profiles for columns of different configuration accomplishing the same separation. Some stages at each end of the column retain roughly the same temperatures for different column configurations; the number is determined by a comparison of the temperature profiles for the first two column calculations. Then for succeeding column configurations, the temperatures of these stages are set at the corresponding temperatures found in the previous column calculation. The temperatures of the remaining stages are estimated by projection from the previously calculated profile for the intermediate stages of the last column configuration; this involves a scaling of the profile from the previous to the new number of stages.

Since reflux will usually be considerably different for different column configurations, with other flows being correspondingly influenced, accurate estimation of new flow profiles can be quite difficult. Also relative changes in the feed location greatly influence the shape of the flow profile so that it is necessary to estimate the profile in each column section separately. Flows are estimated by projection from the liquid flow profiles of the section calculated for the previous column configuration. The estimated rectifying section liquid flows are then multiplied by a scaling factor to force the estimated reflux to correspond to the desired reflux. The stripping section liquid flows are adjusted so that the difference between the estimated liquid flows on the feed stage and the stage above is the same as the corresponding difference in the last calculated liquid profile. The vapor flow profile is simply related to the liquid flow profile through overall material balances, and new composition estimates are directly obtained from solution of component material balances for the estimated temperatures and flows.

#### Convergence Procedures

Successive configurations are examined until values of reflux rate and feed stage composition ratio are within set tolerances of the desired values. These tolerances are put in terms of changes associated with adjustments of one stage in the column. Thus it is required that calculated reflux be such that a change of $n_1$ (usually taken as 1) stages in $N$ will not bring the reflux closer to its specified value, and that $(x_l/x_h)_f$ be such that a change of $n_1$ stages in feed location will not bring it closer to the ratio in feed liquid. This is effected through the requirement that the predicted changes in $N$ and feed location both be less than $n_1/2$. When these conditions are satisfied for any column configuration, one more SC iteration is made and new predicted changes are computed. If one of these is now greater than $n_1/2$, the column configuration must again be corrected. If not, further SC iterations are made for the same configuration until either a predicted change becomes larger than $n_1/2$ or the column calculation reaches a specified final convergence, corresponding to convergence of an operating calculation for the column configuration under consideration. Here this is defined by

$$\left| \sum_{i=1}^{M} y_{ij} - 1 \right| \leq \epsilon \quad \text{for} \quad j = 1, N$$

with a small value for $\epsilon$ ($10^{-3}$ is often sufficient). When

this final convergence is attained, the current column configuration is the design solution. The operation of the convergence procedure is summarized in Figure 2.

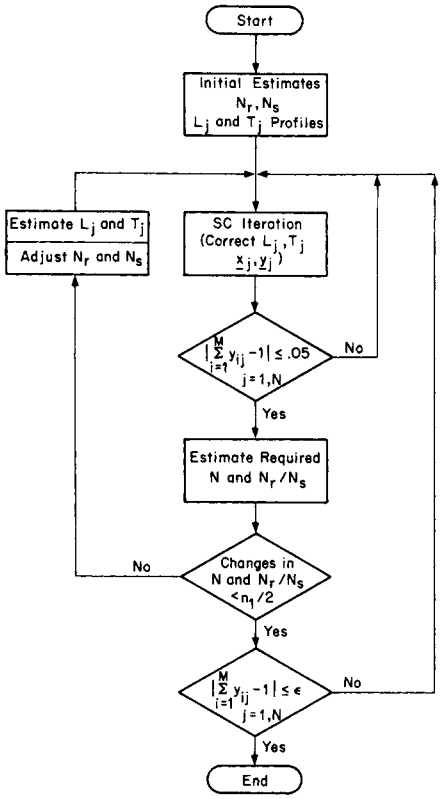


**Fig. 2. DSA correction and convergence procedure.**

## INITIAL ESTIMATES FOR DESIGN CALCULATIONS

For the first column configuration to be examined in a design calculation, estimation of $N$, $N_r/N_s$, and temperature and flow profiles must be made without reference to results for previous configurations. A modified, noniterative, stage-to-stage calculation described by Treybal (1955) seems to give a very satisfactory initial estimate for required stages and column flows. In this method the usual difficulties associated with stage-to-stage methods are avoided because the nonkey components are assumed to be nondistributing and the key components are distributed according to their specified recoveries.

Although the end stage temperatures estimated with this method are also usually satisfactory, the simplifications made often lead to large errors in middle stage temperatures. Therefore, the estimated temperatures of the three stages on each end of the column are used, but the temperatures of the middle stages are initially estimated by linear interpolation between those of the end stages.

## APPLICATION TO SAMPLE PROBLEMS

The DSA procedure has been implemented with a FORTRAN program for the CDC 6400 (Ricker, 1972), and has been applied to a number of design problems encompassing a wide range of characteristics. Very simple relationships were used for calculation of equilibrium and enthalpy values in the interest of reduction of computational expense; however, relationships of any type desired can be easily employed.

Six design problems examined are described in Table 1. Narrow boiling systems are often encountered among critical separation design problems, and Problems A through D are of this nature. Problem E is intermediate, and Problem F is quite wide boiling. Problem A is derived from Holland (1963), while Problem B is based on a debutanizer described by Van Winkle (1967). Problem

TABLE 1. DESIGN PROBLEM SPECIFICATIONS

| Problem | *A* | *B* | *C* | *D* | *E* | *F* |
|---|---|---|---|---|---|---|
| Column pressure, lb/sq.in.abs. | 120 | 85 | 35 | 150 | 300 | 100 |
| Feed composition, mol | | | | | | |
| $C_1$ | | | | | 0.0066 | |
| $C_2=$ | | | | | 0.5461 | |
| $C_2$ | | | | | 0.3041* | |
| $C_3=$ | | | | | 0.0760** | |
| $C_3$ | 0.050 | | | 0.0714 | 0.0480 | 0.240* |
| $iC_4$ | 0.150 | 0.060 | | 0.3864* | | |
| $nC_4$ | 0.250* | 0.170* | 0.0172 | 0.4538** | 0.0115 | 0.060** |
| $iC_5$ | 0.200** | 0.320** | 0.0954* | | | |
| $nC_5$ | 0.350 | 0.450 | | | 0.0077 | 0.080 |
| cis $2C_5$ | | | 0.4102** | | | |
| $3MeC_5$ | | | 0.1241 | | | |
| $nC_6$ | | | | | | 0.050 |
| cis3Me2$C_5$ | | | 0.3340 | | | |
| 33DMe$C_5$ | | | 0.0191 | | | |
| $nC_7$ | | | | | | 0.015 |
| $iC_8$ | | | | 0.0884 | | 0.420 |
| Feed temp., °F | 188.0 | 183.0 | 150.0 | 159.0 | −1.0 | 250.0 |
| Feed B.P., °F | 185.2 | 185.2 | 150.8 | 159.5 | −0.9 | 171.0 |
| Feed D.P., °F | 209.8 | 198.0 | 167.6 | 265.0 | 46.6 | 355.3 |
| Feed vaporization, % | 7.8 | 0 | 0 | 0 | 0 | 21.0 |
| Recovery LK overhead | 0.950 | 0.990 | 0.950 | 0.983 | 0.993 | 0.990 |
| Recovery HK bottoms | 0.950 | 0.990 | 0.994 | 0.941 | 0.900 | 0.950 |
| Multiple of minimum $R$ | 1.20 | 1.24 | 1.55 | 1.33 | 1.05 | 1.30 |

Notes: All problems converged to $n_1 = 1$ stage and $\epsilon = 10^{-3}$ (except for $D$: $\epsilon = 10^{-4}$).
Light Key Component (LK) shown by *.
Heavy Key Component (HK) shown by **.

D represents the deisobutanizer of an alkylation unit (Phillips Petroleum, 1946). Problem E is a deethanizer in an ethylene plant, and Problem F is broadly based on a natural gasoline plant stripper. Problem B was also solved with four arbitrary initial estimates of the column configuration (rather than the estimate calculated by the modified stage-to-stage method) in order to determine the effect of very poor initial estimates on the design calculation procedure. In addition, the problems have been solved as related operating problems by the SC method to provide a basis for comparison of the computational effort required with that required in the design problem solution.

## GENERAL RESULTS

Comparative results for the ten cases studied, including the total number of SC iterations required and the number of column configurations examined by the DSA procedure, are given in Table 2. Also included are the initial and final column configurations. The number of equivalent operating problems solved, as shown in Table 2, is the ratio of design SC iterations to the SC iterations required to solve a closely related operating problem. The initial estimate of the temperatures and flows provided in the solution of this equivalent operating problem was generally better than would be provided in a shotgun approach to a design problem so the number of equivalent operating problems solved is conservatively high in most cases. Problem F was found to be very sensitive to these initial estimates, and a meaningful number of SC iterations for the equivalent operating problem could not be determined. This problem exhibits a large gradient near the feed causing operating calculations to converge slowly from initial linear temperature profiles; it caused no special difficulty in column correction, however.

The initial estimate of the column configuration calculated by the modified stage-to-stage method is usually quite close to the final value obtained, as shown in Table 2 Problems A to F. Given such good initial estimates, it is not surprising that the calculational effort required is low. However, even in cases such as B-1 to B-4, where large errors are deliberately made in the initial estimates used, the DSA procedure is still effective; it has been similarly tolerant of almost any reasonable error in estimates of column stages. The reliability of the design calculation is illustrated by the common solution obtained for Problem B and B-1 to B-4.

The evaluation of the effectiveness of the individual aspects of the DSA procedure requires detailed examination of the iteration results. The important factors are the column configurations selected, the number of SC iterations required for each column calculation, the resulting reflux and feed stage composition ratio, and the predicted correction to $N$ and feed stage location. This information is given in Table 3 for case B-2, which provides a good example of the general behavior of the procedure. The large error in the initial estimate causes initial predicted changes in total stages and feed location to be very large, but these are limited by the procedures described earlier. Note that for most configurations only one SC iteration is required for sufficient accuracy. This indicates that the accuracy of the method for estimation of temperature and flow profiles is adequate. The successive temperature profiles for this case are shown in Figure 3.

Table 2. Design Problem Results

| Problem | *A* | *B* | *B*-1 | *B*-2 | *B*-3 | *B*-4 | *C* | *D* | *E* | *F* |
|---|---|---|---|---|---|---|---|---|---|---|
| SC iterations required by DSA | 4 | 6 | 10 | 13 | 5 | 12 | 4 | 4 | 11 | 14 |
| Column configurations considered | 4 | 3 | 7 | 6 | 5 | 5 | 2 | 2 | 5 | 3 |
| Minimum stages | 9.2 | 11.9 | 11.9 | 11.9 | 11.9 | 11.9 | 29.1 | 25.0 | 7.5 | 7.2 |
| Minimum reflux ratio | 1.9 | 3.4 | 3.4 | 3.4 | 3.4 | 3.4 | 17.2 | 5.1 | 0.28 | 3.4 |
| Initial estimate of $N$ | 17 | 24 | 26 | 26 | 19 | 39 | 44 | 46 | 14 | 11 |
| Final $N$ | 20 | 26 | 26 | 26 | 26 | 26 | 45 | 47 | 17 | 11 |
| Initial estimate $N_r/N_s$ | 6/11 | 7/17 | 16/10 | 2/24 | 5/14 | 10/29 | 22/22 | 17/29 | 6/8 | 2/9 |
| Final $N_r/N_s$ | 8/12 | 8/18 | 8/18 | 8/18 | 8/18 | 8/18 | 22/23 | 17/30 | 7/10 | 3/8 |
| SC iterations for equivalent operating problem | 3 | 5 | 5 | 5 | 5 | 5 | 3 | 3 | 5 | — |
| Computational effort in terms of equivalent operating problems | 1.3 | 1.2 | 2.0 | 2.6 | 1.0 | 2.4 | 1.3 | 1.3 | 2.2 | — |

Table 3. DSA Calculation Behavior for Case *B*-2

Desired reflux ratio = 4.24; Desired $\left(\frac{x_l}{x_h}\right)_f = 0.531$

| Complete iterations | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Configuration: | | | | | | |
| $N$ | 26 | 24 | 32 | 25 | 27 | 26 |
| $N_r/N_s$ | 2/24 | 14/20 | 13/19 | 9/16 | 9/18 | 8/18 |
| SC iterations | 5 | 3 | 1 | 1 | 1 | 2 |
| Reflux ratio | 14.14 | 3.84 | 3.91 | 4.37 | 4.14 | 4.26 |
| $(x_l/x_h)_f$ | 4.40 | 0.462 | 0.454 | 0.443 | 0.478 | 0.513 |
| Predicted change in: | | | | | | |
| Number of stages ($N$) | +11.7 | −1.8 | −6.8 | +1.7 | −.8 | +.3 |
| Feed location ($N_s/N$) | −0.58 | +0.02 | −0.05 | −0.32 | +0.04 | +0.01 |

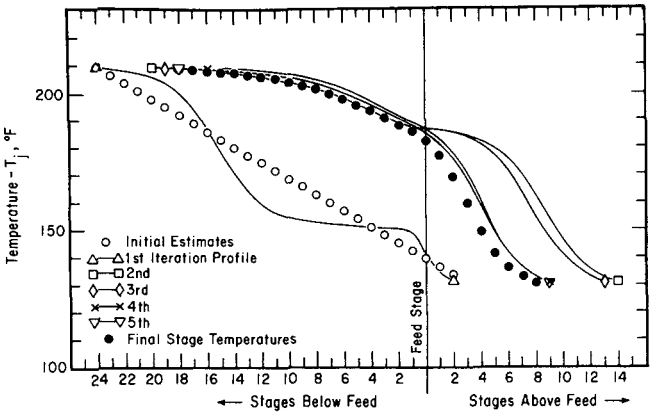


**Fig. 3. Temperature profiles calculated for complete iterations of Case B-2.**

### Computational Efficiency

The computational effort for solution of a design problem by the DSA procedure is seen in Table 2 to be equivalent to that required for about 1.3 to 2.6 operating problems (when solved by an efficient SC method). This is considerably less than would be required for shotgun application of operating calculations to design problems, which, in general, can be expected to need at least 3 or 4 operating solutions, even in the hands of an experienced engineer. Moreover, application of calculational methods for operating problems requires considerable effort in formulation of these problems so as to, in the end, reach one that accomplishes the specified separation. This effort is also avoided by the DSA procedure. Thus this approach to design calculations in multicomponent distillation offers a decided advantage in computational efficiency.

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## NOTATION

$B$ = bottom
$D$ = distillate
$E_1, E_2$ = error parameters for column configuration
$f_{ij}$ = feed of component $i$ to stage $j$
$F_j$ = total feed to stage $j$
$h_{ij}$ = liquid molal enthalpy of component $i$ on stage $j$
$H_{ij}$ = vapor molal enthalpy of component $i$ on stage $j$
$K_{ij}$ = vaporization equilibrium ratio for component $i$ on stage $j$
$L_j$ = liquid flow from stage $j$
$M$ = number of components
$n_1$ = convergence criterion in terms of equivalent change in $N$
$N$ = total number of stages
$N_r$ = number of rectifying stages
$N_s$ = number of stripping stages including feed stage
$r$ = reflux ratio, $R/D$
$R$ = reflux flow
$T_j$ = temperature on stage $j$
$V_j$ = vapor flow from stage $j$
$x_{ij}$ = liquid mol fraction of component $i$ on stage $j$
$y_{ij}$ = vapor mol fraction of component $i$ on stage $j$
$\alpha_{ih}$ = relative volatility of light key with respect to heavy key component
$\gamma$ = $1/(N_r/N_s + 1)$
$\epsilon$ = convergence criterion in terms of error in mol fraction summation
$(/_i)_D$ = recovery fraction for component $i$ in distillate

**Subscripts**

$c$ = calculated
$e$ = estimated
$f$ = feed stage liquid
$F$ = feed liquid
$h$ = heavy key component
$l$ = light key component

**Superscript**

$(r)$ = iteration index

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