A Collocation Approach to Distillation Column Design

A reduced-order collocation method is applied to the optimal design of distillation columns. The resulting number of equations is determined by the user and is independent of the numbers of stages in the column sections. The collocation method furthermore permits these stage numbers to be treated as continuous variables, thus extending the discrete solution set. This greatly facilitates the optimization. Several demonstration problems are worked out.

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Introduction

A major difficulty in the optimal design of distillation columns is the fact that the number of stages is discrete. Optimal design with full-order stagewise models thus requires the solution of a mixed integer nonlinear programming problem. The problem is compounded by the fact that the number of equations varies with the number of stages.

Various solution strategies have been proposed. Brosilow et al. (1968) circumvented the limitation to discrete numbers of stages by defining a new set of difference equations. They did this by reformulating the original problem as a continuous one, and then applying finite-difference approximations with a larger mesh.

Subsequent workers have restricted the number of stages to integer values. Ricker and Grens (1974) proposed an iterative design method involving a succession of loosely converged operating problems with different trial numbers of stages. This method yielded a feasible design, but not necessarily an optimal one, since the feed tray location was determined by a heuristic criterion. Sargent and Gaminibandara (1976) optimized the discrete and continuous variables separately in a pair of nested loops. The feed was distributed to all the stages in proportions determined by the optimization. Holland (1981) included the numbers of stages as integer variables in a direct search optimization method.

In the present paper, the stagewise orthogonal collocation method described by Stewart et al. (1985) is extended to optimal design of distillation systems. The numbers of stages in the column sections are now treated as continuous variables, thus extending the discrete solution set. Distillation design problems are consequently reduced to standard nonlinear programming (NLP) problems, thus greatly facilitating the optimization calculations.

The Stagewise Collocation Method

The stagewise collocation method of Stewart and coworkers (1985) is summarized in this section. The reader is referred to the original paper for a more detailed description of the method.

The fractionation system is represented as a series of interconnected modules such as the one shown in Figure 1. The following conditions are assumed in the present demonstration:

1. Good mixing of the phases on each stage.
2. A given Murphree vapor efficiency for each stage.
3. Thermal equilibrium between the liquid and vapor leaving each stage.
4. No entrainment between the stages.
5. Adiabatic stages.

Under these assumptions, the steady state operation of each module is described by the following equations, commonly referred to as the MESH equations. [MESH = Material balance equations, Efficiency relations, Summation equations, and Heat (enthalpy) balance equations.] Here the stage number s takes integer values from 1 to N.

Material Balance Equations:

$$\underline{\ell}_{s-1} + \underline{v}_{s+1} - \underline{\ell}_s - \underline{v}_s = \underline{0} \tag{1}$$

Stage Efficiency Relations:

$$\underline{y}_s - \underline{y}_{s+1} = \underline{\underline{E}}_{MVs}[\underline{y}_s^*(\underline{x}_s, T_s, p_s) - \underline{y}_{s+1}] \tag{2}$$

where

$$\underline{y}_s = \frac{\underline{v}_s}{V_s}$$

$$\underline{x}_s = \frac{\underline{\ell}_s}{L_s}$$

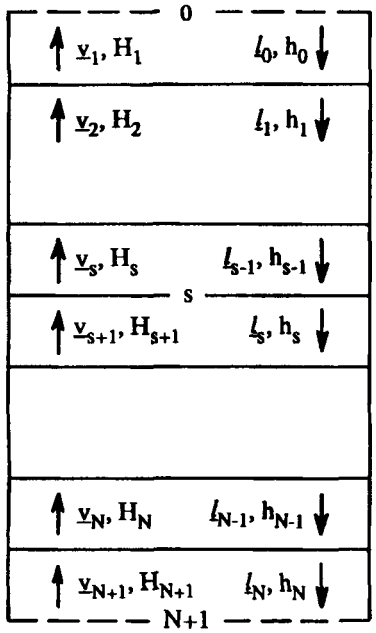

Figure 1. A multistage module.

Summation Equations:

$$L_s = \sum_{i=1}^{c} \ell_{si} \tag{3}$$

$$V_s = \sum_{i=1}^{c} v_{si} \tag{4}$$

Enthalpy Balance Equations:

$$L_{s-1}h_{s-1} + V_{s+1}H_{s+1} - L_s h_s - V_s H_s = 0 \tag{5}$$

Equations 1 to 5 may be used to represent an equilibrium condenser and an equilibrium reboiler by the removal of variables corresponding to a liquid stream above the condenser and a vapor stream below the reboiler, and the inclusion of condenser and reboiler heat duties, Q_C and Q_R, in the respective enthalpy balance equations.

In the collocation method, the stagewise variables in each module are approximated by polynomials using $n \le N$ interior grid points, s_j, along with entry points: $s_0 = 0$ for the liquid states and $s_{n+1} = N + 1$ for the vapor states. Lagrange interpolation of the liquid and vapor flows of components and enthalpy over the module then gives:

$$\underline{\tilde{\ell}}(s) = \sum_{j=0}^{n} W_{\ell j}(s)\underline{\tilde{\ell}}(s_j) \quad 0 \le s \le N \tag{6}$$

$$\underline{\tilde{v}}(s) = \sum_{j=1}^{n+1} W_{vj}(s)\underline{\tilde{v}}(s_j) \quad 1 \le s \le N+1 \tag{7}$$

$$\tilde{L}(s)\tilde{h}(s) = \sum_{j=0}^{n} W_{\ell j}(s)\tilde{L}(s_j)\tilde{h}(s_j) \quad 0 \le s \le N \tag{8}$$

$$\tilde{V}(s)\tilde{H}(s) = \sum_{j=1}^{n+1} W_{vj}(s)\tilde{V}(s_j)\tilde{H}(s_j) \quad 1 \le s \le N+1 \tag{9}$$

with

$$\tilde{L}(s) = \sum_{i=1}^{c} \tilde{\ell}_i(s)$$

$$\tilde{V}(s) = \sum_{i=1}^{c} \tilde{v}_i(s)$$

The W functions in Eqs. 6 to 9 are Lagrange polynomials, given by:

$$W_{\ell j}(s) = \prod_{\substack{k=0 \\ k\neq j}}^{n} \frac{(s - s_k)}{(s_j - s_k)} \quad j = 0, \ldots, n \tag{10}$$

$$W_{vj}(s) = \prod_{\substack{k=1 \\ k\neq j}}^{n+1} \frac{(s - s_k)}{(s_j - s_k)} \quad j = 1, \ldots, n+1 \tag{11}$$

The tilde ($\tilde{}$) is used to indicate an approximating function.

Substitution of the approximating functions into the MESH equations, Eqs. 1–5, yields a corresponding set of residual functions, interpolable as continuous functions of s. The collocation equations are obtained by setting the interpolated residuals to zero at the interior grid points $s_1, \ldots, s_n$:

$$\underline{\tilde{\ell}}(s_j - 1) + \underline{\tilde{v}}(s_j + 1) - \underline{\tilde{\ell}}(s_j) - \underline{\tilde{v}}(s_j) = \underline{0} \quad j = 1, \ldots, n \tag{12}$$

$$\underline{\tilde{y}}(s_j) - \underline{\tilde{y}}(s_j + 1) - \underline{\underline{\tilde{E}}}_{MV}(s_j)[\underline{y}^*(\underline{\tilde{x}}(s_j), \tilde{T}(s_j), \tilde{p}(s_j)) - \underline{\tilde{y}}(s_j + 1)] = \underline{0} \quad j = 1, \ldots, n \tag{13}$$

where

$$\underline{\tilde{y}}(s) = \frac{\underline{\tilde{v}}(s)}{\tilde{V}(s)}$$

$$\underline{\tilde{x}}(s) = \frac{\underline{\tilde{\ell}}(s)}{\tilde{L}(s)}$$

$$\tilde{L}(s_j - 1)\tilde{h}(s_j - 1) + \tilde{V}(s_j + 1)\tilde{H}(s_j + 1) - \tilde{L}(s_j)\tilde{h}(s_j) - \tilde{V}(s_j)\tilde{H}(s_j) = 0 \quad j = 1, \ldots, n \tag{14}$$

Stewart et al. (1985) have shown the appropriate collocation points to be the zeros of the corresponding Hahn polynomial. The Hahn polynomials $Q_n(x; \alpha, \beta, K)$ obey the weighted orthogonality condition

$$\sum_{x=0}^{K} w(x; \alpha, \beta, K)\, Q_m(x; \alpha, \beta, K) \cdot Q_n(x; \alpha, \beta, K) = 0 \quad (m \neq n) \tag{15a}$$

in which

$$w(x; \alpha, \beta, K) = \frac{(\alpha + 1)_x(\beta + 1)_{K-x}}{x!(K - x)!} \tag{15b}$$

The weighting parameters α and β are required to be greater than -1. The choice $(\alpha, \beta) = (0, 0)$ recommended by Stewart et al. gives uniform weighting: $w(x; 0, 0, K) = 1$.

Additional useful properties of this polynomial family, including explicit formulas for the zeros of the first four polynomials with $(\alpha, \beta) = (0, 0)$, are given by Stewart et al. (1985).

Design Problem Statement

The general statement for the optimal design problem is:

$$\begin{aligned} &\text{Minimize:} && \phi(\underline{z}) \\ &\text{Subject to:} && \underline{h}(\underline{z}) = \underline{0} \\ & && \underline{g}(\underline{z}) \geq \underline{0} \end{aligned} \tag{16}$$

where

$\underline{z}$ = vector of model variables
$\underline{h}(\underline{z})$ = MESH equations and equality specifications
$\underline{g}(\underline{z})$ = inequality specifications.

This statement includes the problem of calculating the minimum number of stages to produce a given separation. More generally, the objective function would be a total cost, comprising both capital and operating costs. With the collocation method, the MESH equations are applied at the reduced point set $s_1, \ldots, s_n$ in each module as shown in Eqs. 12 to 14.

The collocation formulation has properties other than that of order reduction, which make it particularly suitable for design calculations:

1. The number of model equations is determined by the number of collocation points, which is independent of the number of stages N (except that n cannot exceed N).

2. The Hahn polynomials are given by explicit formulas, which can be evaluated not only for integer values $N = K + 1$, but also for any real number $N \geq n$. If the domain of N in the collocation method is thus extended, the design problem, Eq. 16, reduces to a standard nonlinear programming problem.

Figure 2 illustrates the variation in collocation point location with the continuous variable N for the third-degree Hahn polynomial $Q_3(s - 1; 0, 0, N - 1)$. The smooth variation of the three collocation points with N permits solution for N by gradient-based techniques. The diagram also illustrates that when the number of collocation points corresponds to the actual number of stages, the collocation points coincide with the stage locations and the full-order model is recovered. In the limit as N becomes

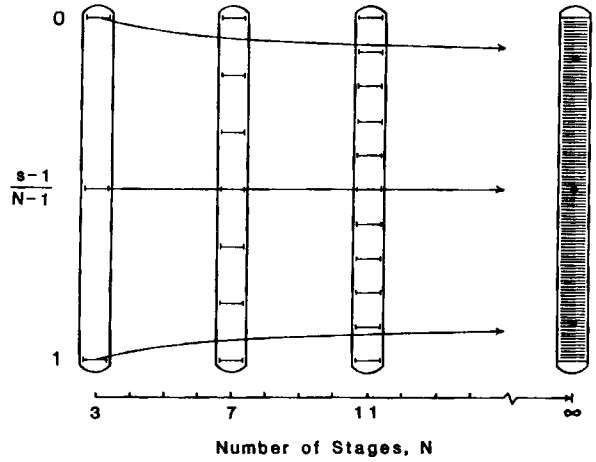

Figure 2. Variation of collocation point locations with number of stages N for $n = 3$.

Let $\underline{z} = \begin{bmatrix} \underline{u} \\ --- \\ \underline{x} \end{bmatrix}$

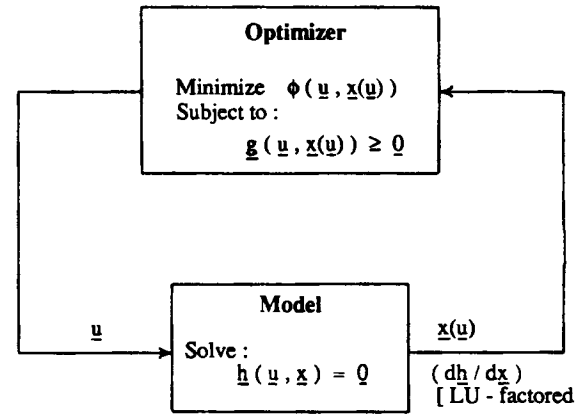

Figure 3. Design solution strategy.

infinite, the collocation points coincide with the zeros of the corresponding Jacobi polynomial, appropriate for models continuous in s, as for packed columns.

Solution Strategy

A modular solution strategy for Eq. 16 is illustrated in Figure 3. The variables are partitioned into a set of decision or input variables and a set of dependent variables. The optimization is carried out over the space of decision variables, with the dependent variables calculated by solution of the equality constraints. The model and optimizer can thus be considered as separate entities. The inequality constraints are included in the optimizer. If the model equations are solved by Newton's method, the gradient information required by the optimizer can be obtained with relative ease by use of the LU-factored Jacobian at the model solution.

For illustrative purposes, the problems discussed in this paper are confined to a conventional distillation column with an equilibrium condenser and an equilibrium reboiler, such as the column illustrated in Figure 4. The following quantities are assumed to be specified:

1. Feed composition, flow rate, temperature, and pressure
2. Column pressure
3. Stage efficiencies.

The system is then described by $(n_1 + n_2 + 2)(2c + 1)$ collocation equations in an equal number of grid-point variables (temperatures, and liquid and vapor component flows) along with four system variables: N_1, N_2, Q_C, and Q_R. N_1 and N_2 are the numbers of stages in the rectifying and stripping sections, respectively, while n_1 and n_2 are the respective numbers of collocation points in these modules. The module entrance conditions are obtained by simple material and energy balances around the module junctions and do not appear explicitly in the main equation system.

Four additional specifications are thus required to obtain a solution. Common choices are four members from the set

$$S = \{N_1, N_2, D, R, d_{lk}/f_{lk}, b_{hk}/f_{hk}\}$$

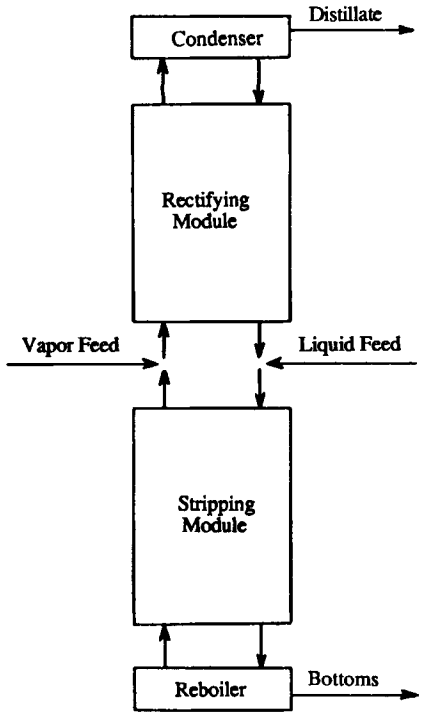

Figure 4. Modules assembled to form a conventional distillation column.

where the ratios d_{lk}/f_{lk} and b_{hk}/f_{hk} are light and heavy key component recovery fractions. The designer is by no means restricted to the indicated list; other specifications may be used as long as they yield a well-conditioned problem.

Specification of N_1 or N_2 removes the corresponding variable from the set of unknowns. Specifications of distillate flow rate, reflux ratio, and key component recovery fractions, on the other hand, provide the following additional relationships between the unknowns:

$$D = \sum_{i=1}^{c} v_{C,i} \tag{17}$$

$$R = \frac{\sum_{i=1}^{c} \ell_{C,i}}{\sum_{i=1}^{c} v_{C,i}} \tag{18}$$

$$d_{lk}/f_{lk} = \frac{v_{C,lk}}{f_{lk}} \tag{19}$$

$$b_{hk}/f_{hk} = \frac{\ell_{R,hk}}{f_{hk}} \tag{20}$$

These latter quantities are conveniently considered as variables in the system of model equations augmented by Eqs. 17 to 20.

Certain members of the selected four specifications are fixed in the problem statement, while the remaining members become the decision variables $\underline{u}$ indicated in Figure 3. The solution setup in any given case is conveniently represented by a diagram such as Figure 5. The set S is thus partitioned into:

- Decision variables
- Quantities that are fixed throughout the calculation

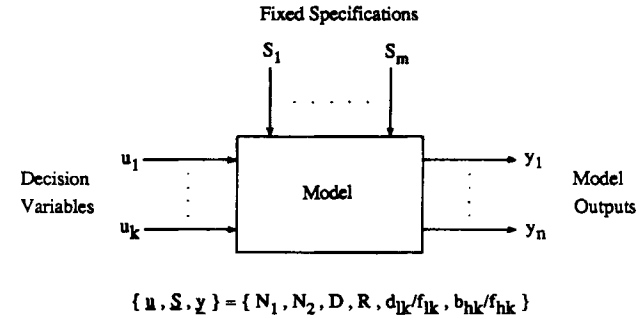

Figure 5. Model solution scheme.

- Dependent quantities that are obtained from the model solution.

The four specifications from the set S must be carefully chosen. Only those combinations of specification variables that result in a well-posed problem are permitted. For example, the specifications D, d_{lk}/f_{lk} and b_{hk}/f_{hk} give linearly dependent equations in binary separations, and ill-conditioned ones in multicomponent problems.

Minimum-Stage Design

The problem of calculating the minimum number of stages for a given separation is now considered. Typical specifications are the reflux ratio and the light and heavy key recovery fractions; the resulting optimization problem has one degree of freedom. A convenient choice for the decision variable is N_1 or N_2. Figure 6 illustrates the solution scheme for this problem with N_1 as the decision variable.

The strategy in Figure 6 is possible only if N_1 and N_2 are treated as continuous variables, since integer numbers of stages cannot be directly calculated from the model equations. The restriction to integer-valued numbers of stages would place a lower bound of two on the dimensionality of the optimization, with both N_1 and N_2 necessarily included as decision variables.

Two examples have been included to demonstrate the performance of the proposed approach in minimizing the total number of stages. Binary systems were chosen and constant molal overflow was assumed to permit comparison with the results of a McCabe-Thiele construction. The systems considered were benzene-toluene and *i*-butane–*n*-butane. Ideal solution behavior was assumed, with fugacity data taken from Prausnitz et al. (1980). The problem specifications are listed in Table 1.

The model equations were solved by a damped Newton method. The damping was implemented by halving the Newton corrections until the residual Euclidean norm was reduced below

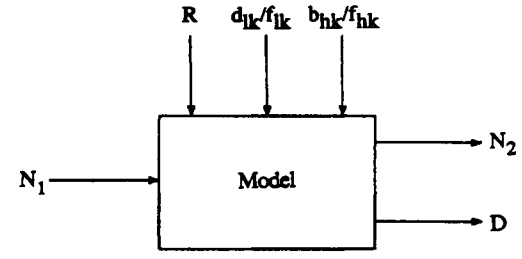

Figure 6. Model solution scheme for minimizing total number of stages.

Table 1. Test Problem Specifications

	Problem No.		
	1	2	3
	No. of Components		
	2	2	5
Feed, mol frac.	Benzene 0.45 Toluene 0.55	i-C4 0.45 n-C4 0.55	C2 0.03 C3 0.20 (*lk*) C4 0.37 (*hk*) C5 0.35 C6 0.05
Total feed, kmol/h	1	1	1,361
Feed temp, °C	166	−5	107
Condenser type	Equil.	Equil.	Equil.
Reboiler type	Equil.	Equil.	Equil.
Pressure, MPa	0.5	0.1	1.723
Distillate, kmol/h	—	—	308
Reflux ratio	2.0883	3.9977	—
d_{lk}/f_{lk}	0.9385	0.9384	≥0.9548
b_{hk}/f_{hk}	0.9596	0.9596	≥0.9832

lk, light key component; *hk*, heavy key component

that obtained in the previous iteration. The golden section search was used for the optimization.

The collocation solutions obtained using various orders of approximation, n, are given in Tables 2 and 3, together with the results of the McCabe-Thiele method. The collocation points used were the zeros of the corresponding Hahn polynomial with $(\alpha, \beta) = (0, 0)$. For ease of comparison, specifications were chosen such that the McCabe-Thiele construction would yield an integral number of stages.

The collocation results are seen to be very good. Sufficiently accurate designs are obtained with four collocation points in each column section. As expected, the accuracy of the collocation results increases with the number of grid points used.

Optimal Economic Design

The objective function to be minimized in the optimal economic design problem is:

ϕ = Annual operating cost + Annualized capital cost

We consider the solution of this problem with specifications of the distillate flow rate and lower bounds for the recovery fractions of the light and heavy key components. Since the recovery fractions are specified by inequalities, they are not incorporated into the model equations, but appear as optimization constraints. The number of degrees of freedom is thus three for the standard column shown in Figure 4. Convenient choices for the decision variables are N_1, N_2, and R. The calculation scheme is illustrated in Figure 7.

Table 2. Results of Problem 1

Collocation Points per Section	Calc. No. of Stages		
	N_1	N_2	$N_1 + N_2$
3	13.21	15.84	29.05
4	11.95	14.85	26.80
5	12.12	14.88	27.00
McCabe-Thiele solution	12	15	27

Table 3. Results of Problem 2

Collocation Points per Section	Calc. No. of Stages		
	N_1	N_2	$N_1 + N_2$
3	21.74	24.17	45.91
4	20.13	22.65	42.78
5	20.27	22.72	42.99
McCabe-Thiele solution	20	23	43

The above calculation was carried out for a five-component system originally studied by Amundson and Pontinen (1958) as an operating problem, and later by Brosilow and coworkers (1968) as a design problem. In the present version, the former workers' thermodynamic data were used, together with the cost data supplied in Appendix A. Variable overflow was included.

The design specifications are listed in Table 1. The problem was solved with five collocation points in each section, obtained as zeros of the Hahn polynomial, $Q_5(s - 1; 0, 0, N - 1)$. Powell's (1977) successive quadratic programming (SQP) algorithm was used for the optimization. The model equations were solved by the damped Newton method described in the previous section. The problem was solved in seven iterations of the SQP algorithm with initial values of 15, 15, and 4.0 for N_1, N_2, and R, respectively. The results are shown in Table 4. The light-key recovery constraint is binding at the optimum, and the heavy-key constraint is slack.

For comparison, the full stagewise optimum was also determined. This was done by specifying various combinations of integral numbers of stages, and optimizing the reflux ratio for each configuration. The resulting objective function values are tabulated in Table 5 as a function of the numbers of stages in each section. The optimal case found by this exhaustive search is closely approximated by the collocation solution in Table 4.

Conclusions

The number of equations used in reduced-order collocation is independent of the numbers of stages in the column sections. The method furthermore permits these numbers to be treated as continuous variables without losing the stagewise character of the model. The new formulation consequently reduces distillation design problems to standard nonlinear programming (NLP) problems, for which a number of efficient solution techniques exist.

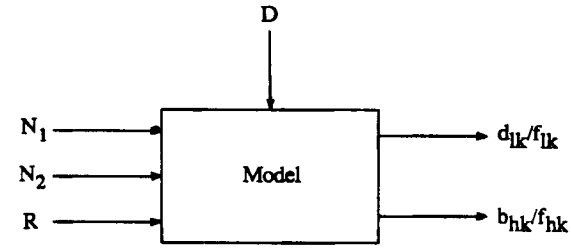

Figure 7. Model solution scheme for optimal economic design.

Table 4. Collocation Solution to Problem 3

N_1	13.15
N_2	18.10
Reflux ratio	3.8960
d_{lk}/f_{lk}	0.9548
b_{hk}/f_{hk}	0.9865
Total annual cost	\$203,048

lk, light key component; *hk*, heavy key component

The commonly considered problem of minimizing the total number of stages to produce a specified separation at a given reflux ratio can consequently be solved as a univariate optimization problem. The collocation procedure also permits efficient calculation of optimal economic designs in which both capital and operating costs are considered. While the latter type of optimization typically involves additional degrees of freedom, the continuous stage numbers permit the use of rapidly convergent gradient-based optimization techniques.

While only one solution procedure for the NLP problem is demonstrated here, the method is quite general with regard to the choice of NLP optimization algorithm. The structure of the formulation furthermore permits direct extension to complex distillation systems.

Acknowledgment

The authors are pleased to acknowledge useful discussions with Arthur W. Westerberg, and with Ross E. Swaney, who provided a code for the Powell SQP algorithm. This work was supported by Grant No. DE-FG02-84ER13291 of the U.S. Department of Energy, Division of Chemical Sciences (Office of Basic Energy Sciences).

Notation

b_{hk}/f_{hk} = recovery fraction of heavy key component in bottoms
c = number of components
D = distillate molar flow rate, kmol/h
d_{lk}/f_{lk} = recovery fraction of light key component in distillate
$\underline{\underline{E}}_{MV}$ = Murphree vapor efficiency matrix
$\underline{f}$ = vector of feed component flows, kmol/h
$\underline{g}$ = inequality constraints
$\underline{h}$ = equality constraints
$\bar{h}$ = liquid molar enthalpy
H = vapor molar enthalpy
K = upper limit of x in Eq. 15a
$\underline{\ell}$ = vector of liquid component flows, kmol/h
$\underline{\ell}_C$ = vector of liquid component flows from condenser
$\underline{\ell}_R$ = vector of liquid component flows from reboiler
$\bar{L}$ = liquid molar flow rate, kmol/h
n = degree of polynomial; number of collocation points in module
n_1 = value of n in rectifying module
n_2 = value of n in stripping module
N = module length (stages)
N_1 = length of rectifying module
N_2 = length of stripping module
p = pressure at mass transfer interface
Q_C = condenser heat duty, kJ/h
Q_R = reboiler heat duty, kJ/h
$Q_n(x; \alpha, \beta, K)$ = nth degree Hahn polynomial
R = reflux ratio
s = stage coordinate
s_j = jth collocation point in module
T = temperature
$\underline{v}$ = vector of vapor component flows, kmol/h
$\underline{v}_C$ = vector of vapor component flows from condenser
$\bar{V}$ = vapor molar flow rate, kmol/h
$W_{\ell j}(s)$ = Lagrange polynomial for liquid states

Table 5. Total Annual Costs in Problem 3, Calculated from Full-order Model

	N_1		
N_2	12	13	14
17	\$203,216	\$202,962	\$202,985
18	\$203,094	\$202,840 (optimum)	\$202,862
19	\$203,124	\$202,869	\$202,890
	R (optimum) = 3.8875		

$W_{vj}(s)$ = Lagrange polynomial for vapor states
x = coordinate in Hahn polynomials
$\underline{x}$ = liquid composition vector
$\underline{y}$ = vapor composition vector
$\underline{y}^*(\underline{x}, T, p)$ = vapor bubble point composition corresponding to liquid state $(\underline{x}, T, p)$
α, β = weighting parameters in Hahn polynomials
ϕ = objective function

Subscripts

i = ith component
s = stage s

Operations

$\tilde{f}(s)$ = continuous approximation to the constants f_s
$(a)_k = (a)(a+1)\ldots(a+k-1)$ if $k > 0$
$(a)_k = 1$ if $k = 0$

Appendix A. Cost Data for Problem 3

ϕ = Annual operating cost + Annualized capital cost

Operating cost = $(Q_C)(C_1) + (Q_R)(C_2)$

where

Q_C = condenser duty

Q_R = reboiler duty

C_1 = (\$0.322/million kJ)(8,640 h/yr)

C_2 = (\$0.790/million kJ)(8,640 h/yr)

Capital cost = $(C_3)(N_1 + N_2 + 2)$

where

$$C_3 = (118.752 + 360.2D + 368.1D^2 - 1.438D^3 + 28.78D^4)/10$$

D is the column diameter in meters, calculated to yield a top-stage superficial vapor velocity of 0.127 m/s.

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Manuscript received Mar. 6, 1986, and revision received April 7, 1986.