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Distillation Column Simulation by Orthogonal Collocation: Efficient Solution Strategy

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Abstract. A reduced-order collocation method (using Jacobi or Hahn polynomials) is used for the simulation of distillation columns. A new solution strategy which uses the overall balances and equilibrium relations to eliminate the need to include the vapour flows approximating profiles from the solution algorithm is presented. Furthermore the material balance equations are included in the enthalpy balance equations to improve convergence. The proposed strategy is compared against a formerly published basic strategy and is shown to offer a considerable saving in computer time.

Nomenclature

A_j, B_j, C_j	Coefficients of liquid enthalpy collocation (see equation (8)) in units of Btu, Btu/°F and Btu/(°F)^2 respectively.
a_j, b_j, c_j	Coefficient of vapor enthalpy correlation (see equation (9)) in units of Btu, Btu/°F and Btu/(°F)^2 respectively.
C	Number of components, dimensionless.
d_j, D	Distillate molar flow rate of component j and of total flow respectively, lb.mol/hr.
E_{MV}	Murphree plate efficiency at collocation points
$H_{s,i}{}^s$	Vapour enthalpy of a component at collocation point s_i, Btu/lb.mole.
$h_{s,j}$	Liquid enthalpy of a component at collocation point s_j, Btu/lb.mole.
$K_{s,j}$	Equilibrium constant of a component at collocation point s_j, dimensionless.
$l_{s,j}$	Liquid molar flow rate of a component at collocation point s_j, lb.mol/hr.
$L(s_j)$	Total liquid molar flow rate, lb.mol/hr.

N	Plates number in a rectifying or stripping section.
$P_j(x)$ and $Q_j(x)$	Polynomials in x.
s_j	Collocation point j.
T_s	Temperature at stage s, °F.
$T_{s,j}$	Temperature at collocation point s_j, °F.
$v_{s,j}$	Vapour molar flow rate of component j, lb.mol/hr.
$V_{s,j}$	Total vapour molar flow rate at collocation point s_j, lb.mol/hr.
x	Independent co-ordinate, e.g. dimensionless distance.
f_j	Computed liquid flow rate of component j, lb.mol/hr.
$x_{s,j}$	Liquid mole fraction of component j at stage s, dimensionless.
$y_{s,j}$	Vapour mole fraction of component j at stage s, dimensionless.
$y^*_{s,j}$	Equilibrium vapour mole fraction of component j at stage s, dimensionless.
y	Dependent variable, e.g. molar flow rate, lb.mol/hr.
F_j	Exact liquid flow rate of component j, lb.mol/hr.
α, β	Parameters in the weighting functions required for the orthogonality of Jacobi and Hahn polynomials.
$\alpha_j, \beta_j, \gamma_j, \delta_j$	Coefficients of equilibrium constant correlation.

Introduction

The present study involves a reduced-order approach to the simulation of distillation columns. Full order simulation of multi-stage separation schemes usually lead to large systems of nonlinear algebraic or stiff differential equations [1]. The design, control and optimization studies for such problems would be greatly facilitated if the system of equations for such problems can be reduced to a simpler form. Furthermore, the reduction of the dimensionality of staged separation processes models is a necessity if the real time dynamic simulation of such complex processes is to be realized [2]. Thus a real-time simulator (used for control room operators training for example) can be made to simulate abnormal working conditions. The orthogonal collocation method is a mathematical technique which can be used for this purpose.

Earlier collocation methods presented in the literature used collocation points based on Jacobi polynomials to describe plate columns [3,4]. Such a choice of collocation points is unsuited to the discrete nature of plate column models [1]. Stewart, *et al.* [1] gave a reduced-order collocation method suitable for plate columns, and Swartz and Stewart [5] adapted the method to optimal column design.

In this work, the authors propose the comparison of the model reduction procedure on the basis of two different solution strategies. The two strategies are applied to a specific example and their accuracies compared. The effect of the choice of the

number of collocation points, the approximating polynomial and the weighting function on the solution efficiency are examined.

Problem Statement

Figure 1 shows a distillation column consisting of a rectifying section, a stripping section, a reboiler, a condenser (which can be a total or an equilibrium partial condenser) and a single feed stream. The following assumptions are made:

1. Good mixing of each phase on each stage.
2. Thermal equilibrium between the liquid and vapour effluents from each stage.
3. Each stripping or rectifying stage is adiabatic.

A traditional full order rigorous, multicomponent approach for the modelling of such a column would establish a set of MESH (for Material, Equilibrium, Summation and Heat) equations for each stage in the column. The ensuing set of simultaneous non-linear equations would then be solved by one computational method or another [6].

In the collocation method approach the number of such equations is vastly reduced by assuming that the vapour and liquid component flows as well as enthalpies (or temperatures) inside each section of the column can be approximated by polynomials. The resulting number of equations is determined by the user and is independent of the actual numbers of plates in the column sections. The user is thus free to choose the number of collocation points in each section (where each collocation point corresponds to a hypothetical plate on which the MESH relationships apply) and the type of polynomial to use to approximate the system profiles inside the column. The number of collocation points chosen, however, can never exceed the actual number of stages in the given region. The accuracy of the model thus obtained will largely depend on the number of collocation points and the type of approximating polynomial used. Furthermore, as outlined later in this paper, the manner in which the material, energy and equilibrium relationships are combined and presented can also affect the accuracy as well as speed of computations.

With reference to Fig. 1, the fresh feed can be a single or two-phase feed. Entering collocation stages in the rectifying section can be interstage liquid from collocation stage (s-1) above of molal flow rates $l_{s-1,j}$ and enthalpy $h_{s-1,j}$ and temperature $T_{(s-1)}$. The subscript j refers to component j. Similarly, from stage (s+1) below interstage vapour of molal flow rates $v_{s+1,j}$ enthalpy $H_{s+1,j}$ and temperature T_{s+1} can enter stages. Leaving stage s is vapour of molal flow rates $v_{s,j}$ and temperature T_s and this stream constitutes an interstage stream to be sent to stage (s-1) above. Also a liquid stream of molal flow rates $l_{s,j}$ and temperature T_s leaves stage s to enter stage (s+1) below. Note that streams V_s and L_s are in thermal equilibrium. Compo-

nent flow rates have been used instead of the cumbersome combination of total flow rates and mole fractions. A similar arrangement is used in the stripping section. The feed plate is considered as an equilibrium stage where the fresh feed (whether one or two-phase feed) is mixed with the liquid from the bottom plate of the rectifying section and the vapour from the top plate in the stripping section. A vapour stream leaves the feed plate and enters the bottom plate of the rectifying stream while liquid stream leaves the feed plate and enters the top plate of the stripping section.

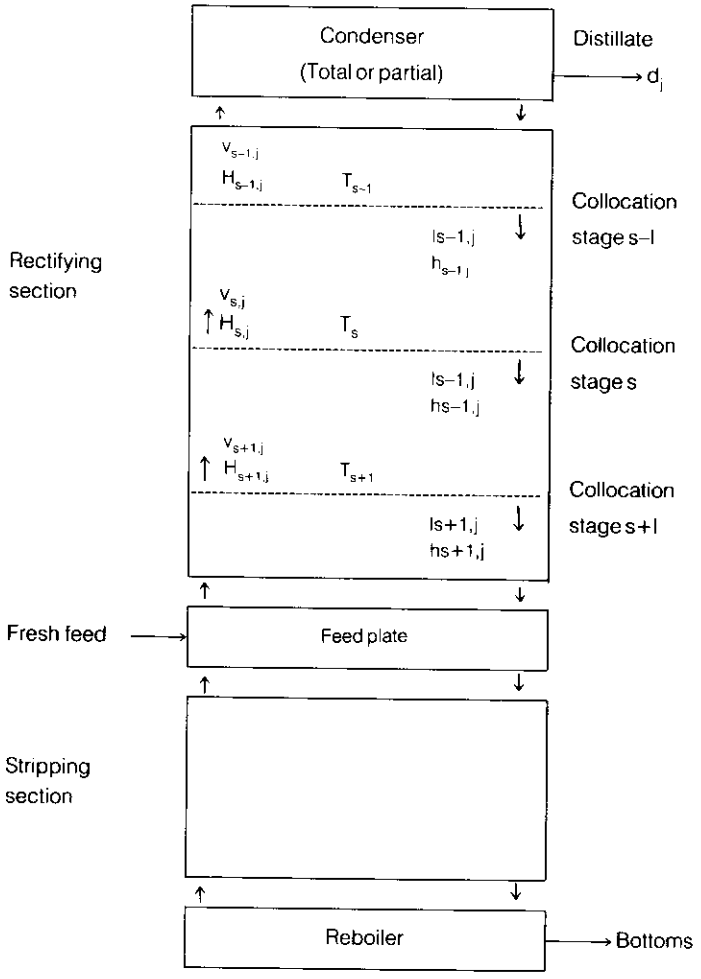

Fig. 1. Distillation column

For the system described, the MESH equations are given by,
Material Balance Equations:

$$l_{s-1,j} + v_{s+1,j} = l_{s,j} + v_{s,j} \tag{1}$$

Stage Efficiency Relations:

$$y_{s,j} - y_{s+1,j} = e_{MV_s} [y^*_{s,j} - y_{s+1,j}] \tag{2}$$

where

$$y^*_{s,j} = k_{s,j}\, x_{s,j}$$

$$y_{s,j} = \frac{v_{s,j}}{v_s}$$

$$x_{s,j} = \frac{l_{s,j}}{l_s}$$

Summation Equations:

$$L_s = \sum_{j=1}^{C} l_{s,j} \tag{3}$$

$$V_s = \sum_{j=1}^{C} v_{s,j} \tag{4}$$

Enthalpy Balance Equations:

$$\sum_{j=1}^{C} l_{s-1,j}\, h_{s-1,j} + \sum_{j=1}^{C} v_{s+1,j}\, H_{s+1,j} = \sum_{j=1}^{C} l_{s,j}\, h_{s,j} + \sum_{j=1}^{C} v_{s,j}\, H_{s,j} \tag{5}$$

Few modifications are needed in these equations for a condenser, reboiler and feed plate. For an equilibrium condenser remove variables corresponding to a liquid stream above the condenser and include condenser heat duty in the enthalpy balance equations. For a reboiler remove vapour stream below the reboiler and include reboiler heat duty in the enthalpy balance equations. For a feed plate include feed flow rate and its enthalpy in the corresponding material and heat balance equations.

Approximating Polynomials

The orthogonal collocation method is suitable for the solution of two point non-linear boundary value problems. To solve such a system (described by either differential or algebraic equations), this technique assumes that the dependent variables (component flow rates, concentrations or temperatures inside a distillation column for example) can be approximated by polynomial functions of the independent variables, so that the equations describing the system are satisfied at certain points of the interval being studied. Such points are called collocation points. In the present study two intervals are considered: The first between the feed plate and condenser and the second between the feed plate and reboiler.

The flows of material and enthalpy in each interval were approximated by Lagrange polynomials, whose nodal values were determined by orthogonal collocation at the zeros of a Hahn polynomial [1] or a Jacobi polynomial [1,4]. The basic features of the collocation method are outlined here and for full details the reader is referred to [1] or [5].

Each state is expressed as a trial function (Y) which is taken as an expansion of orthogonal polynomials.

The Jacobi polynomials P_i satisfy the continuous orthogonality condition:

$$\int_0^1 x^{\beta} (1-x)^{\alpha} P_i(x) P_j(x) \, dx = 0 \qquad (6)$$

$$\begin{aligned} &i = 0,1, \ldots, M \\ &j = 0,1, \ldots, M \\ &i \neq j \\ &\alpha, \beta > -1 \\ &0 \leq x \leq 1 \end{aligned}$$

The Hahn polynomials Q_i satisfy the discrete orthogonality condition

$$\sum_{y=0}^{M} \frac{(\alpha+1)_{(M-y)} (\beta+1)_y}{y! \, (M-y)!} Q_i(xM) Q_j(xM) = 0 \qquad (7)$$

$$;x = \frac{y}{M} \qquad \begin{array}{l} i = 0,1,\ldots, M \\ j = 0,1,\ldots, M \\ i \neq j \\ \alpha, \beta > -1 \\ 0 \leqslant x \leqslant 1 \end{array}$$

$$\text{where } (a)_k = a(a+1)\ldots(a+k-1) \qquad \text{if } k > 0$$
$$= 1 \qquad \text{if } k = 0$$

where (a) refers to $(\alpha+1)$ or $(\beta+1)$ and k refers to (M–y) or y.

The software package supplied in Villadsen and Michelsen [7] contains the subroutines JCOBI and INTRP. Subroutine JCOBI is used in this study for the computation of the JACOBI polynomials zeros.

As an illustration, let Y(s) represent a trial function of the approximate solution for an n point collocation scheme. Then

$$Y(s) = \sum_{j=1}^{n} \prod_{\substack{i=1 \\ j \neq i}}^{n} \frac{(s - s_i)}{(s_j - s_i)} Y(s_j) \tag{8}$$

Subroutine INTRP computes the coefficients of the solution polynomial as a vector XINTP. Thus the output vector for any specified value of s is:

$$XINTP(i) = \prod_{\substack{i=1 \\ j \neq i}}^{n} \frac{(s - s_i)}{(s_j - s_i)} \tag{9}$$

the approximate solution Y(s) is then computed from:

$$Y(s) = \sum_{j=1}^{n} XINTP(j) * Y(s_j) \tag{10}$$

where $Y(s_j)$ is the exact value of the polynomial at collocation point s_j

Example problem

Figure 2 shows the specifications and overall results of a fractionator [8]. It is required to determine the liquid composition profiles of the five components inside

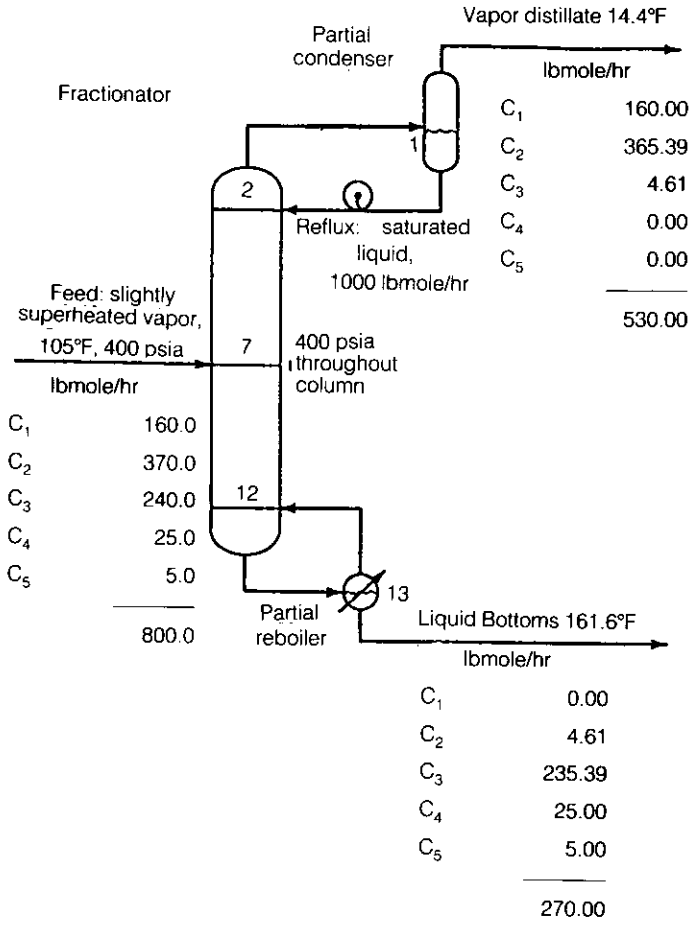

Fig. 2. Column specifications of the illustrative example [8]

the column. Equilibrium stages are assumed such that $E_{MV_s} = 1$. The problem has been solved [8] using one of the full-length traditional computational methods (the computer program of Johansen and Seader based on the Wang-Henke procedure [6] was used for this problem). The full-length computations involved making initial assumptions for the distillate and bottoms temperatures and then go through a number of iterative solutions until a specified convergence criterion is met [6].

In this study the collocation approach is applied using two different solution strategies A and B. Each strategy involves a different combination of material, energy and equilibrium relationships. The two solution strategies and their computational efficiencies are as follows:

Solution strategy "A"

This strategy is suggested by Stewart et al.[1], in each section of the fractionation tower the following equations were developed:

A component material balance round collocation stage s gives:

$$l_{s,j} + v_{s,j} = l_{s-1,j} + v_{s+1,j} \tag{11}$$

An enthalpy balance round collocation stage s gives:

$$\sum_{j=1}^{5} l_{s,j}\, h_{s,j} + \sum_{j=1}^{5} v_{s,j}\, H_{s,j} = \sum_{j=1}^{5} l_{s-1,j}\, h_{s-1,j} + \sum_{j=1}^{5} v_{s+1,j}\, H_{s+1,j} \tag{12}$$

Where $H_{s,j}$ and $h_{s,j}$ refer to the component specific enthalpies of the vapour and liquid phases respectively and are expressed as functions of the temperature T_s on stage s as follows [6]:

$$H_{s,j} = A_j + B_j T_s + C_j T^2_s \tag{13}$$

$$h_{s,j} = a_j + b_j T_s + c_j T^2_s \tag{14}$$

Since the liquid and vapour phases are assumed to be in equilibrium, we obtain for stage s the following equilibrium relationship:

$$\frac{v_{s,j}}{\sum_{j=1}^{5} v_{s,j}} = K_{s,j} \left(\frac{l_{s,j}}{\sum_{j=1}^{5} l_{s,j}}\right) \tag{15}$$

The equilibrium constant $K_{s,j}$ is a function of the temperature T_s at stage s as follows [6]:

$$K_{s,j} = \alpha_j + \beta_j T_s + \gamma_j T^2_s + \delta_j T^3_s \tag{16}$$

Additional component material balances and equilibrium relationships are established round the condenser, feed plate and reboiler. An enthalpy balance round the feed plate is also made.

In this strategy, the component flow rates and enthalpies are approximated by

$$l(s) = \sum_{j=0}^{n} W_{l_j}(s)\, l_{s_j} \qquad 0 \leq s \leq N \qquad (17)$$

$$v(s) = \sum_{j=1}^{n+1} W_{v_j}(s)\, v_{s_j} \qquad 1 \leq s \leq N+1 \qquad (18)$$

$$h(s) = \sum_{j=0}^{n} W_{l_j}(s)\, h_{s_j} \qquad 0 \leq s \leq N \qquad (19)$$

$$H(s) = \sum_{j=1}^{n+1} W_{v_j}(s_j)\, H_{s_j} \qquad 1 \leq s \leq N+1 \qquad (20)$$

where

$$W_{l_j}(s) = \prod_{\substack{k=0 \\ k \neq j}}^{n} \frac{(s - s_k)}{(s_j - s_k)} \qquad j = 0, \ldots, n$$

$$W_{v_j}(s) = \sum_{\substack{k=1 \\ k \neq j}}^{n+1} \frac{(s - s_k)}{(s_j - s_k)} \qquad j = 1, \ldots, n+1$$

At a collocation point s_j we have

$$l(s_j - 1) + v(s_j + 1) = l(s_j) + v(s_j) \qquad (21)$$

$$\frac{v(s_j)}{V(s_j)} = K(s_j) \frac{l(s_j)}{L(s_j)} \qquad (22)$$

$$\sum_{j=1}^{5} l(s_j - 1)\, h(s_j - 1) + \sum_{j=1}^{5} v(s_j + 1)\, H(s_j + 1) = \sum_{j=1}^{5} l(s_j)\, h(s_j) + \sum_{j=1}^{5} v(s_j)\, H(s_j) \qquad (23)$$

where the summation is over the number of components.

Number of equations = 11 n equations in rectifying section
+ 11 n equations in stripping section
+ 10 equations for the condenser

+ 10 equations for reboiler
+ 11 equations for feed plate
+ 1 equation for distillate specification
+ 1 equation for reflux specification
+ 1 equation for temperature equivalence for vapour and liquid leaving feed plate.

Total = 22 n + 34.

In this case the interior collocation points are obtained from the formula.

$$s_j = 1 + x_j (N-1)$$

where x_j,s are the roots of Jacobi polynomials or Hahn polynomials for M = N–1, and N is the number of plates in a particular section of the column. In addition to these interior collocation points, the boundary point $s_0 = 0$ is included for the liquid state and $s_{n+1} = N+1$ for the vapour state.

For solution strategy "A" the total number of algebraic equations to be solved are 56, 78 and 100 equations for 1, 2 and 3 collocation points in each section respectively.

Solution strategy "B"

The following strategy is suggested in this work to reduce the number of equations to be solved.

In this strategy overall material and heat balances equations are used in addition to those at collocation points. In adition, the overall balance is used to express the vapour component flow rates entering and leaving stage s as a function of the relevant liquid component flow rates, the distillate component flow rates and the equilibrium constants.

Figure 3 shows a section of the rectifying section over which an overall component balance is established.

Overall component balances give:

$$\sum_{j=1}^{5} v_{s+1,j} = \sum_{j=1}^{5} l_{s,j} + \sum_{j=1}^{5} d_j \qquad (24)$$

$$\sum_{j=1}^{5} v_{s,j} = \sum_{j=1}^{5} l_{s-1,j} + \sum_{j=1}^{5} d_j \qquad (25)$$

Equilibrium relationships give:

$$\frac{v_{s+1,j}}{\sum_{j=1}^{5} v_{s+1,j}} = K_{s+1,j}\left(\frac{l_{s+1,j}}{\sum_{j=1}^{5} l_{s+1,j}}\right) \tag{26}$$

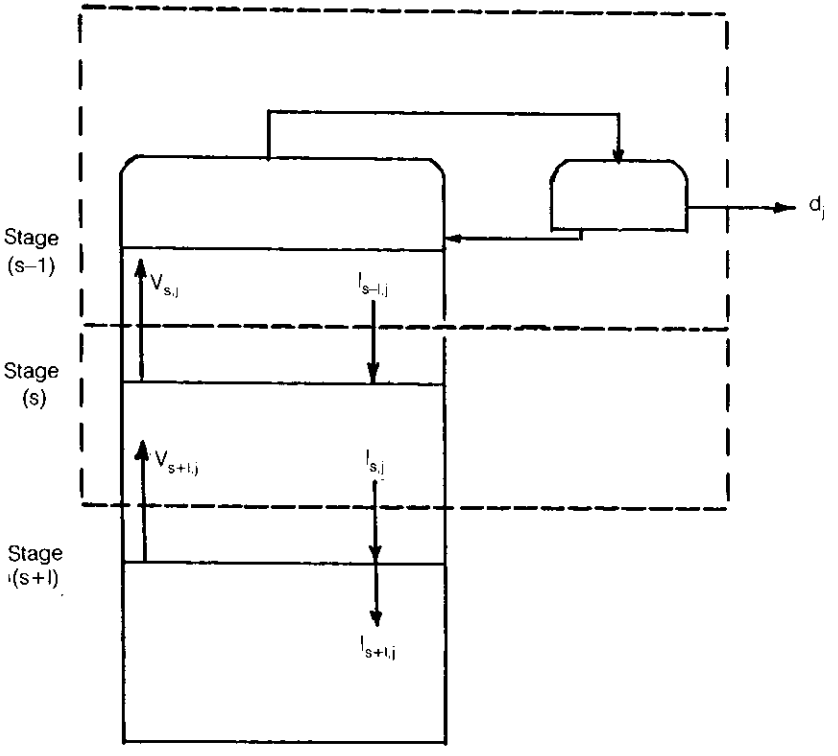

Fig. 3. Balances over sections of the rectifying section

substituting for $\sum_{j=1}^{5} v_{s+1,j}$ from equation (24) we obtain:

$$v_{s+1,j} = K_{s+1,j}\left(\frac{l_{s+1,j}}{\sum_{j=1}^{5} l_{s+1,j}}\right)\left(\sum_{j=1}^{5} l_{s,j} + \sum_{j=1}^{5} d_j\right) \tag{27}$$

Similarly we obtain a relationship for $v_{s,j}$:

$$v_{s,j} = K_{s,j}\left(\frac{l_{s,j}}{\sum_{j=1}^{5} l_{s,j}}\right)\left(\sum_{j=1}^{5} l_{s-1,j} + \sum_{j=1}^{5} d_j\right) \tag{28}$$

Thus the vapour component flow rates entering and leaving stage s have been expressed in terms of liquid component flow rates. After substitution of (27) and (28) into (21), the component material balance equations will no longer contain vapour flow rates. This procedure eliminates the need to include the vapour approximating profile from the solution algorithm.

In the stripping section the overall component balances include the bottom component flow rates instead of the distillates.

An additional distinction between strategies "A" and "B" is that in strategy "B" the material balance equations are included in the enthalpy balance equations to improve convergence. Thus in strategy "B", the liquid component flow rates and temperatures are approximated by:

$$l(s) = \sum_{j=0}^{n+1} W_{l_j}(s)\, l(s_j) \qquad 0 \leq s \leq N \tag{29}$$

$$T(s) = \sum_{j=0}^{n+1} W_{l_j}(s)\, T(s_j) \tag{30}$$

where

$$W_{l_j}(s) = \prod_{k=0}^{n+1} \frac{(s - s_k)}{(s_j - s_k)} \qquad j=0, \ldots, n+1$$

At a collocation point s_j, we have:

$$l(s_j-1) + K(s_j+1)\frac{l(s_j+1)}{L(s_j+1)}[L(s_j) + D] = l(s_j) + K(s_j)\frac{l(s_j)}{L(s_j)}[L(s_j-1) + D] \tag{31}$$

$$\sum l(s_j-1)\, h(s_j-1) + \sum\left[K(s_j+1)\frac{l(s_j+1)}{L(s_j+1)}\right]\,[L(s_j+D)]\, H(s_j+1) = \sum l_{s_j}\, h(s_j)$$

$$+ \sum \left\{ \left[l(s_j - 1) + K(s_j + 1) \frac{l(s_j + 1)}{L(s_j + 1)} [L(s_j) + D] - l(s_j) \right] [H(s_j)] \right\} \qquad (32)$$

Notice that the enthalpy balance as written above is obtained by the substitution of material balances in the enthalpy balance of the original equations. This manipulation is found to improve the convergence of the resulting non-linear equation to the solution.

Number of equations	= 6 n	(rectifying section)
	+ 6 n	(stripping section)
	+ 10	(condenser)
	+ 5	(reboiler)
	+ 6	(feed plate)
	+ 1	(distillate)
	+ 1	(reflux)
	+ 1	(temperature equivalence)
	+ 6	(equations for overall mass and heat balance in the rectifying section)
	+ 6	(similar equations for stripping)

Total number of equations = 12 n + 36.

In this case the interior collocation points are calculated from

$$s_j = 1 + x_j (N - 2)$$

where x_j,s refer to the roots of the Jacobi polynomials or Hahn polynomials for M = N–1.

The boundary points $s_0 = 0$ and $s_{n+1} = N + 1$ are also included in the interpolating polynomial.

The total number of algebraic equations to be solved are 48 and 60 equations for 1 and 2 collocation points in each section respectively.

Comparison of Results

The liquid mole fractions profiles of components C_1 to C_4 are plotted against stage numbers. Component C_5 mole fractions are negligible throughout the column. Figs 4, 5 and 6 show the liquid component mole fractions according to solution strategy A for 1, 2 and 3 collocations in each section respectively. Figs 7 and 8 are the corresponding figures for one and two collocations points respectively according to strategy B.

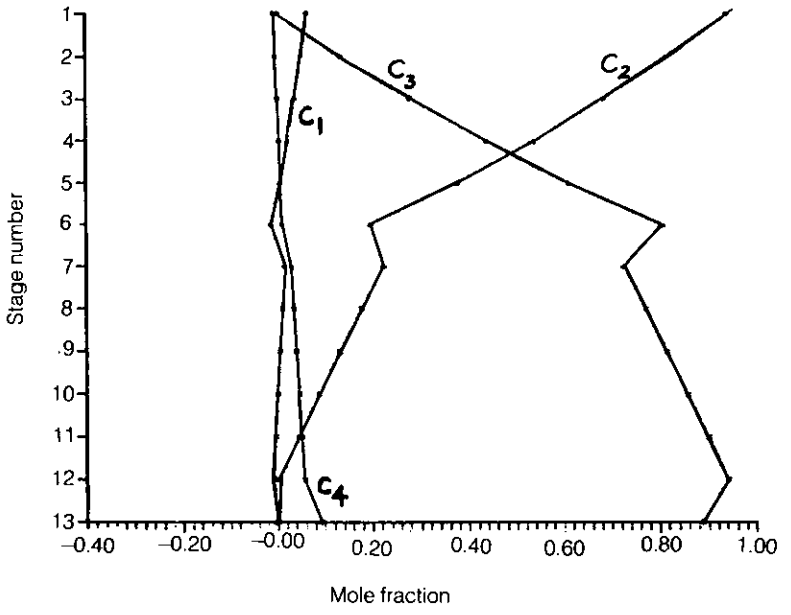

Fig. 4. **Liquid mole fraction profiles (strategy A, one collocation point, Jacobi, $\alpha = 0$, $\beta = 0$)**

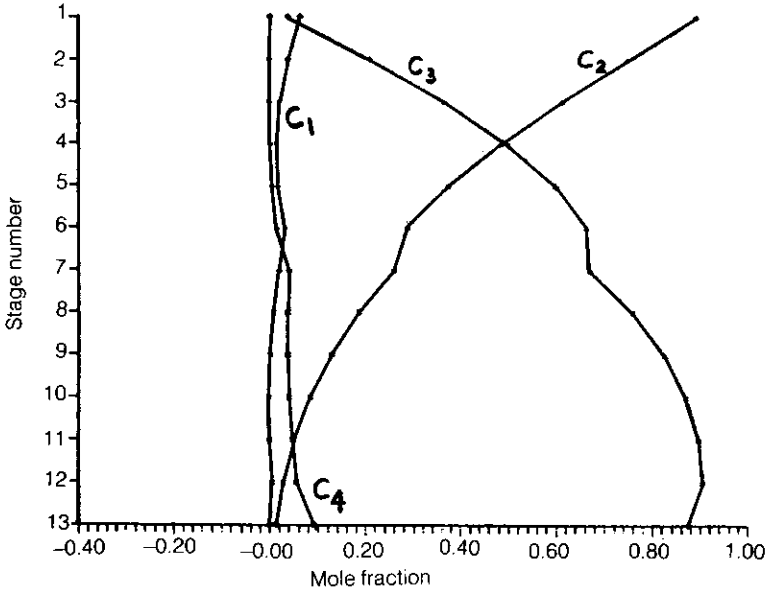

Fig. 5. **Liquid mole fraction profiles (strategy A, two collocation points, Jacobi, $\alpha = 0$, $\beta = 0$)**

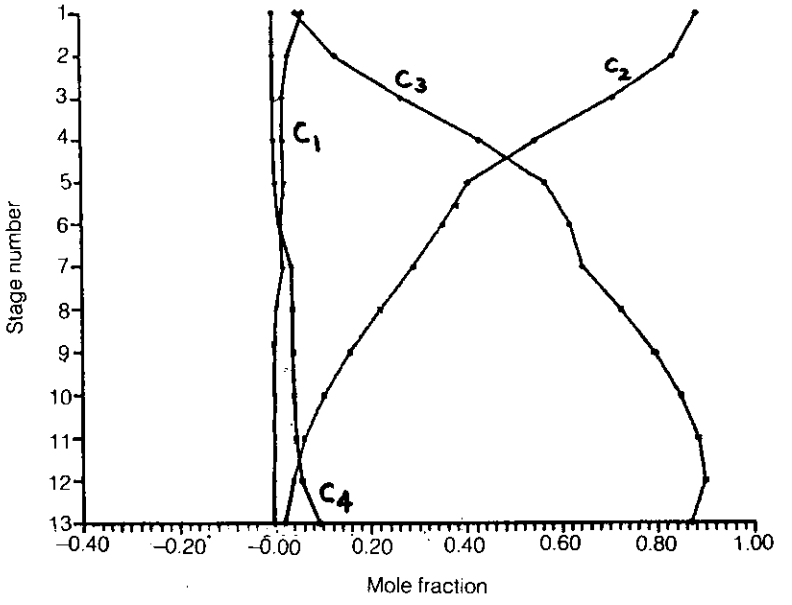

Fig. 6. **Liquid mole fraction profiles (strategy A, three collocation points, Jacobi, $\alpha = 0$, $\beta = 0$)**

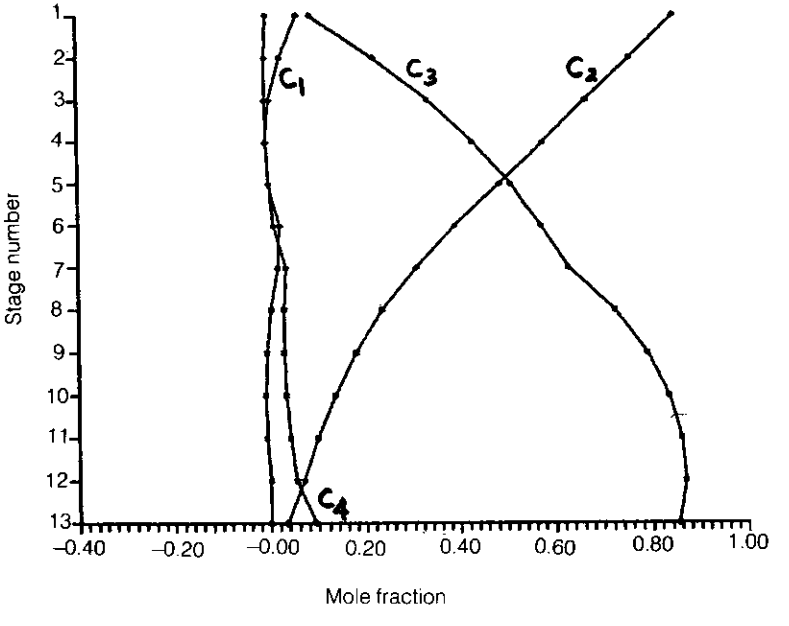

Fig. 7. **Liquid mole fraction profiles (strategy B, Jacobi, $\alpha = 0$, $\beta = 0$)**

The exact solutions as computed by the traditional full order methods is given in Henley and Seader [8] and are shown in Fig. 9. Fig. 10 shows the exact solutions as computed by the orthogonal collocation method (a Hahn polynomial for strategy B is used) when using a number of collocation points equal to the actual number of plates in each distillation column section (5 in this case).

A qualitative assessment of these figures shows that three collocation points according to strategy A and two according to strategy B per column section are needed to give a very close simulation of the exact results. However in order to give a quantitative assessment we use the mean root square difference for this purpose. If f_j and F_j represent the component computed and exact values of the liquid flow rates on any plate then the expression:

$$\sum_{j=1}^{5} (f_j - F_j)^2/5$$

is used as a measure of the deviation of the approximate solution from the exact solution on each plate. As a measure of speed of computations the number of iterations until convergence is obtained is also evaluated. The number of iterations is defined as the number of times the subroutine ZSPOW IMSL calls the functions subroutine. The ZSPOW IMSL subroutine is based on a Newton-Raphson method in which the Jacobian is evaluated numerically. Thus the number of iterations as defined here does not only include the function evaluations required by a Newton-Raphson step but also include the function for Jacobian estimation. Table 1 gives the results of these computations. It is clear from this table that solution strategy A (with n=3) is slightly closer to the exact solution than solution strategy B (with n=2). However solution strategy B converges to its final solution much faster. Taking the sum of the mean square error for all stages as a numerical indicator of accuracy, it is clear from Tables 1 and 2 that the best results are obtained using strategy A (α=0, β=0, Hahn) then strategy A (α=0, β=1, Hahn) and strategy B (α=0, β=0, Hahn).

Figures 11, 12 and 13 show the temperature profile inside the column according to the exact solution, strategy (A) and strategy (B) respectively.

Polynomial and α and β parameters testing

Solution strategies A (with N=3) and B (with N=2) are compared for accuracy and speed of computation for different combinations of α and β values for both Jacobi and Hahn polynomials. The results of these computations are shown in Table 2.

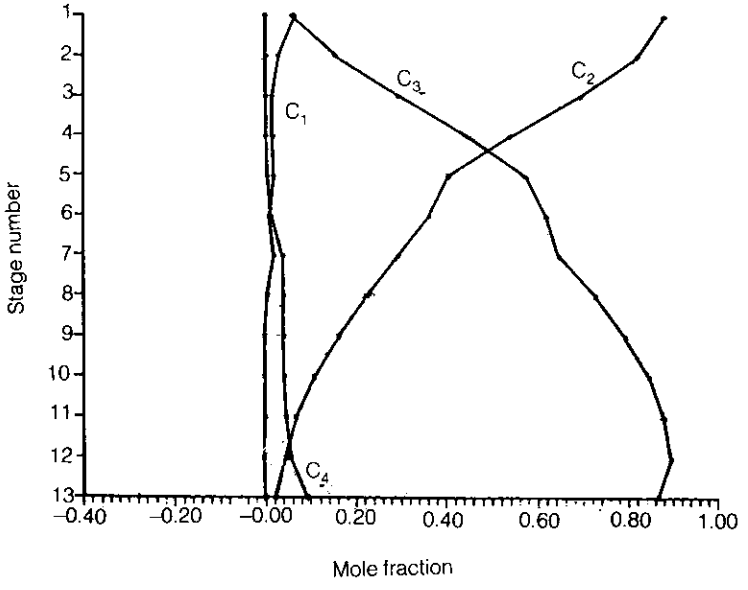

Fig. 8. **Liquid mole fraction profiles (strategy B, Jacobi, $\alpha = 0$, $\beta = 0$)**

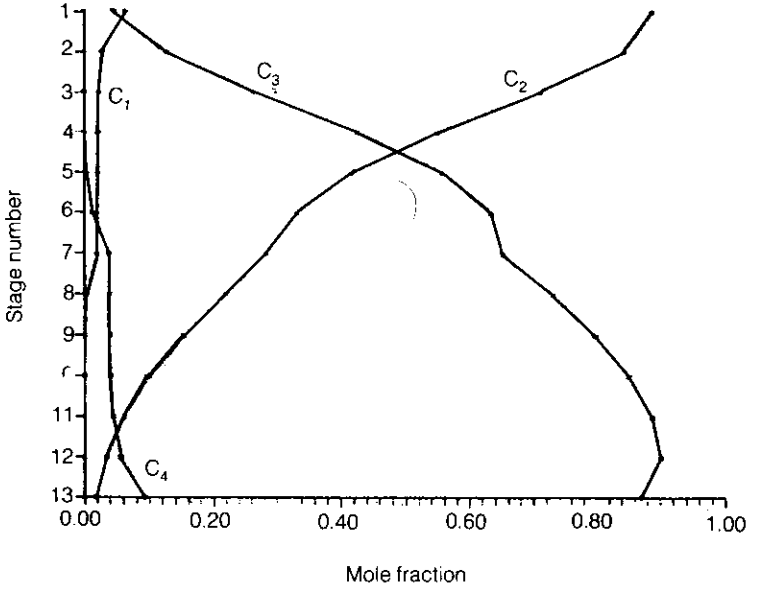

Fig. 9. **Liquid mole fraction profiles (strategy B, Hahn, $\alpha = 0$, $\beta = 0$)**

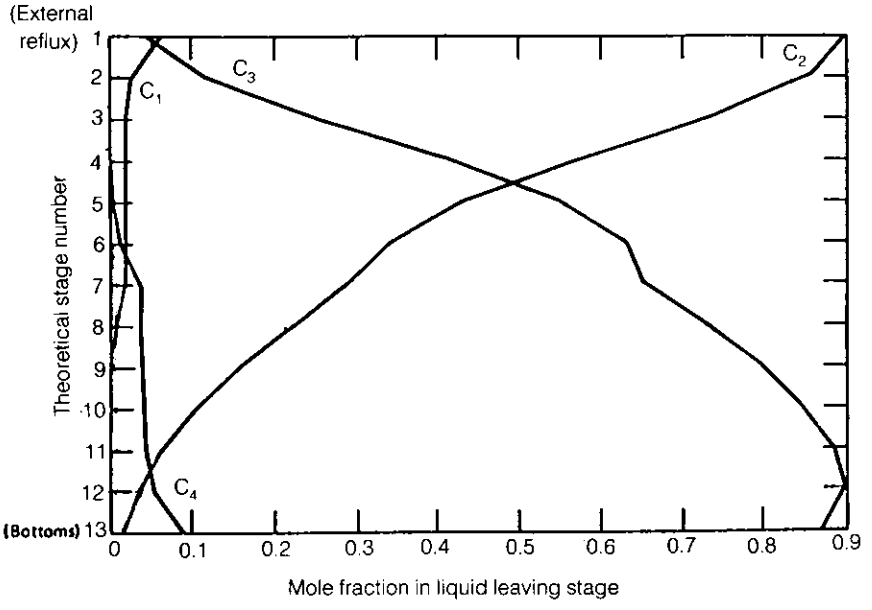

Fig. 10. Converged liquid composition profiles

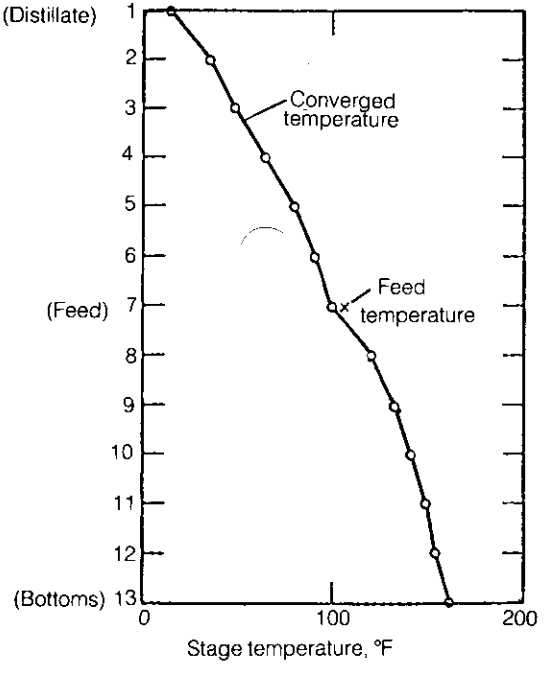

Fig. 11. Exact temperature profile

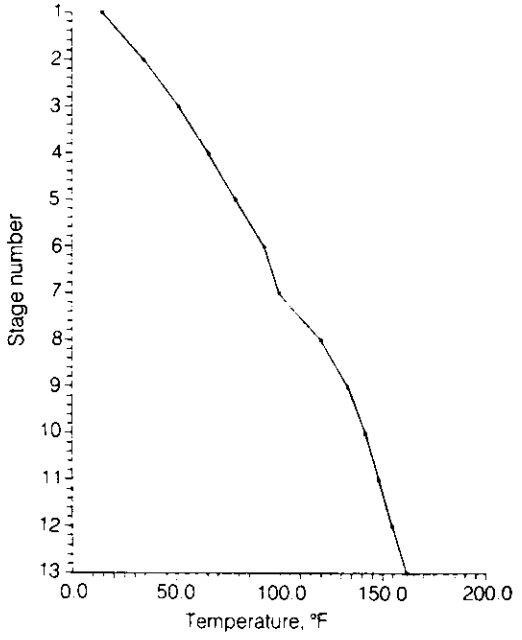

Fig. 12. Temperature profile (strategy A, $\alpha = 0$, $\beta = 0$, Hahn polynomial)

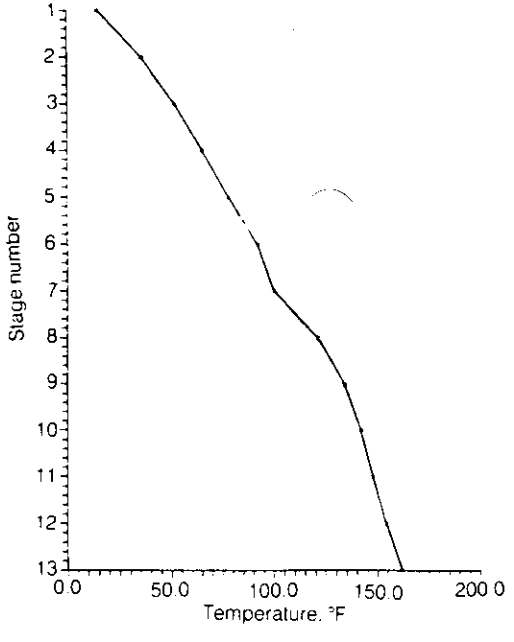

Fig. 13. Temperature profile (strategy B, $\alpha = 0$, $\beta = 0$, Hahn polynomial)

Table 1. Assessment of deviation from exact solution ($\alpha=0$, $\beta=0$ Jacobi polynomial)

$$\sum_{j=1}^{5} (f_j - F_j)^2/5$$

	Strategy (A)			Strategy (B)	
Number of collocation points	n=1	n=2	n=3	n=1	n=2
Total no. of simultaneous equations to be solved	56	78	100	48	60
Number of iterations	64	93	213	57	67
Plate Number:					
13	1.24083	0.26685	0.12001	1.35820	0.37230
12	12.88810	2.51800	0.77640	6.53522	2.04492
11	5.38902	4.65382	1.24987	7.83360	1.31318
10	3.04718	7.09136	1.18881	10.59228	1.74887
9	4.71113	8.34420	1.39061	10.76649	1.89069
8	9.52009	8.03287	1.59199	7.68014	1.27440
7	15.86429	4.79387	1.82183	5.69138	1.97264
6	32.74671	10.08578	4.23199	14.32099	6.52520
5	11.26999	10.48259	2.93856	17.91449	3.72001
4	3.10336	16.90112	0.82818	14.67507	4.75323
3	6.74697	26.22004	0.78490	16.37281	6.66295
2	9.09902	26.28052	3.21909	23.98929	8.22625
1	13.19402	2.09706	0.98551	12.04120	3.26106
Total	128.82072	127.76808	21.12775	149.77116	43.76568

Table 2. Polynomial and parameter testing

	$\sum_{j=1}^{5} (f_j - F_j)^2/5$							
	Strategy (A)						Strategy (B)	
Polynomial	**Jacobi**	**Jacobi**	**Jacobi**	**Jacobi**	**Hahn**	**Hahn**	**Hahn**	**Hahn**
α	0	1	1	0	0	0	0	0
β	1	0	1	2	0	1	0	1
Total no. of simultaneous equations to be solved	100	100	100	100	100	100	60	60
Number of iterations	219	313	315	329	121	223	66	66
Plate No.								
13	0.01011	0.35060	0.18192	0.14561	0.01892	0.06713	0.04652	0.02478
12	0.95137	1.81595	1.09796	0.67401	0.21344	0.46180	0.26479	0.56697
11	1.21665	0.99444	1.45301	1.38597	0.81951	0.75356	0.75993	0.91218
10	0.79618	1.55288	1.46900	2.39755	0.53153	0.54826	0.27989	0.52955
9	1.05782	2.50459	1.77523	3.49133	0.61496	0.87986	0.73970	0.87885
8	1.80610	3.09574	2.14442	4.34842	0.56380	0.69244	1.08233	0.49003
7	0.60301	3.88984	2.69452	3.25087	0.36651	0.82803	1.13990	0.55477
6	0.38817	11.13613	6.34422	6.20716	0.82203	2.77229	2.58361	2.45932
5	5.63412	6.59133	4.05735	13.58660	2.99184	4.65232	5.47969	6.40719
4	6.91177	8.28282	4.27697	21.40129	1.31057	1.34002	0.17755	2.57384
3	10.22003	7.81365	5.00874	29.46690	2.20216	1.05796	2.55301	1.15549
2	11.64670	7.28865	6.47455	27.50720	1.11951	1.48143	0.78662	0.65422
1	0.39709	2.96558	1.50808	1.73821	0.13847	0.52759	0.39890	0.13715
Total	41.63912	58.28218	38.48597	115.60112	11.71327	16.06267	16.29244	17.34434

The tests of strategy A revealed that the Hahn polynomial gives better results than the Jacobi polynomial (for the same combination of α and β) in terms of both accuracy and speed of computation. The best overall results for this strategy are obtained for a combination of $\alpha=0$, $\beta=0$ using the Hahn polynomial. Using the Hahn polynomial, strategy B (with $\alpha=0$, $\beta=0$) proved to be almost as accurate as strategy A (with $\alpha=0$, $\beta=0$ using Hahn polynomial) but at a much enhanced speed of computation. It should be pointed out however that speed of computation is not directly comparable from the number of iterations indicated in Table 2 because the two solution strategies have different number of dependent variables and thus each solution strategy computations were initialized with a different set of initial guesses.

Conclusions

The computational effort involved in distillation column design and simulation can be greatly reduced by using the collocation technique rather than a full-order traditional approach. The number of simultaneous algebraic equations used in the collocation approach is independent of the actual number of plates and is far less than the corresponding number of equations to be solved in the traditional approach. In the demonstration problem used the number of equations [which was 144 equations by the full order method] is reduced to 100 equations by strategy A ($n=3$) which represents a 30.5% reduction and 60 equations by strategy B ($n=2$) which represents a 58.3% reduction. The Hahn polynomial proved to be better suited for this type of discretized staged process equipment. The best overall results are obtained using strategy B with $\alpha=0$, $\beta=0$.

Future work will be concerned with improving the strategy for the solution of the set of non-linear algebraic equations and for treating the cases of steep profiles using spline collocation methods.

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محاكاة برج التقطير بطريقة التنظيم المتعامد
استراتيجية حل متطورة

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ملخص البحث. لقد استخدمت في هذا البحث طريقة تنظيم قليلة الأبعاد (وتشمل متعددتي الحدود جاكوبي أو هان) في محاكاة أبراج التقطير. وقد تم تطوير استراتيجية جديدة باستخدام الموازنات العامة وعلاقات التوازن للاستغناء عن الاستعانة بالمعادلات التقريبية لتدفقات البخار.

وبالإضافة إلى ذلك تم دمج معادلات موازنات المادة في معادلات موازنات الطاقة لتحسين سرعة الوصول إلى الحل الدقيق. وقد أظهرت مقارنة الاستراتيجية المقترحة مع استراتيجية منشورة إلى أن الاستراتيجية المقترحة تحقق وفرًا في وقت الحاسب الآلي.