Finite-Element Steady State Simulation of Multiphase Distillation

A finite-element method is given for efficient simulation of multiphase distillation systems. Breakpoints are adaptively located to coincide with phase discontinuities. Thermodynamic criteria for the states at these discontinuities are included in the equation system. The adjustable breakpoint locations are calculated simultaneously with the other system variables by global Newton iteration. Worked examples demonstrate the accuracy and efficiency of the method.

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Introduction

The presence of more than one liquid phase within a distillation column is generally undesirable because of the uncertainty of the locations of the multiphase regions and the possible maldistribution of liquid and vapor flows. Such operations nevertheless occur industrially. Heterogeneous azeotropic distillation operations fall into this category when the multiphase region extends from the decanter to the upper trays of the column. Accurate prediction of the phase pattern is thus of great importance to determine conditions under which the extent of multiphase regions could be minimized, or to determine locations within the column that would be suitable for sidestream withdrawal and separation.

Figure 1 depicts a single stage on which two liquid phases, I and II, are present. The following conditions are assumed:

1. Good intraphase mixing on each stage
2. Given Murphree vapor efficiencies for each stage
3. Thermal equilibrium between the phases leaving each stage
4. No vapor or liquid entrainment
5. Adiabatic stages

Under these assumptions, the steady state performance of each stage is described by the following equations:

Material Balances

$$L^{\mathrm{I}}_{s-1}\underline{x}^{\mathrm{I}}_{s-1} + L^{\mathrm{II}}_{s-1}\underline{x}^{\mathrm{II}}_{s-1} + V_{s+1}\underline{y}_{s+1} - L^{\mathrm{I}}_{s}\underline{x}^{\mathrm{I}}_{s} - L^{\mathrm{II}}_{s}\underline{x}^{\mathrm{II}}_{s} - V_{s}\underline{y}_{s} = \underline{0} \quad (1)$$

Stage Efficiency Relations

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

$$\underline{y}_s - \underline{y}_{s+1} = \underline{\underline{E}}^{\mathrm{II}}_{MVs}[\underline{y}^*_s(\underline{x}^{\mathrm{II}}_s, T_s, p_s) - \underline{y}_{s+1}] \quad (3)$$

Summation Equations

$$\sum_{i=1}^{c} y_{s,i} = 1 \quad (4)$$

$$\sum_{i=1}^{c} x^{\mathrm{I}}_{s,i} = 1 \quad (5)$$

$$\sum_{i=1}^{c} x^{\mathrm{II}}_{s,i} = 1 \quad (6)$$

Energy (Heat) Balance

$$L^{\mathrm{I}}_{s-1}h^{\mathrm{I}}_{s-1} + L^{\mathrm{II}}_{s-1}h^{\mathrm{II}}_{s-1} + V_{s+1}H_{s+1} - L^{\mathrm{I}}_{s}h^{\mathrm{I}}_{s} - L^{\mathrm{II}}_{s}h^{\mathrm{II}}_{s} - V_{s}H_{s} = 0 \quad (7)$$

While the above equations constitute a straightforward extension of the usual MESH equations for a stage with one liquid and one vapor phase, there is an inherent difficulty in their solution. Equations 1–7 are always satisfied by a degenerate solution, with two identical liquid phases and zero total flow of one of them. A well-posed formulation thus requires either prior knowledge of the phase pattern or, more generally, the inclusion of thermodynamic stability criteria. A common solution procedure is to do the stability testing and phase pattern adjustment in an outer iteration loop.

Block and Hegner (1976) were among the first to describe the solution of distillation problems involving a second liquid phase. They solved the column equations by a tearing procedure in which the mean of the liquid compositions on each stage was computed in an outer iteration loop, whereas the remaining variables were adjusted in inner loops. The authors did not describe the procedure used for determining the number of liquid phases on each stage.

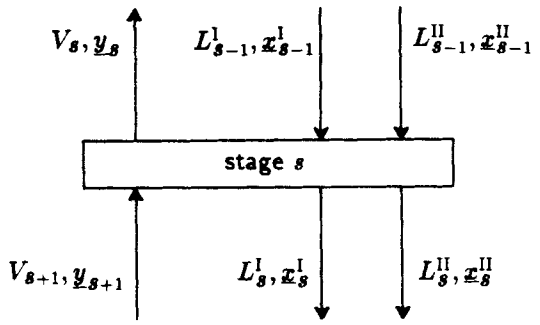

Figure 1. Single stage with two liquid phases.

Boston and Shah (1979) extended the "inside-out" algorithm of Boston and Sullivan (1974) to accommodate two liquid phases. Their method is an equation-tearing procedure in which parameters of approximate thermodynamic models are used as outer loop iteration variables. A stability test to determine the expected number of liquid phases was included in the outer loop.

Ross and Seider (1981) proposed an algorithm for three-phase distillation systems that involved the use of approximate thermodynamic models and the phase-splitting algorithm of Gautam and Seider (1979a,b). Prokopakis et al. (1981) adapted the method to simulation of azeotropic systems.

Buzzi Ferraris and Morbidelli (1981) analyzed three-phase distillation systems by Newton iteration on the full set of model equations, and also by an equation-tearing procedure. The column phase pattern was updated by performing a series of single-stage flash calculations. Buzzi Ferraris and Morbidelli (1982) gave a simplified model for systems in which one of the liquid phases is nearly pure.

In the present paper a collocation method is developed for distillation systems containing regions with differing numbers of liquid phases. The phase miscibility boundaries are included as unknowns in the system of column equations. These locations are calculated simultaneously with the other system variables, thus greatly facilitating the solution of such systems. The method is shown to give highly accurate approximations.

Collocation Procedure

Stewart et al. (1985) developed a stagewise orthogonal collocation method for rapid, accurate simulation of distillation systems. The fractionation system was represented as a series of interconnected modules, each of which corresponded to a physical column section. The states in each module were approximated by Lagrange polynomials whose nodal values were determined by orthogonal collocation. The method was extended by Swartz and Stewart (1986) to the efficient design of distillation systems by treating the module lengths as continuous variables.

The collocation method is readily extended to multiphase systems. A separate module, or finite element, is used to represent each multiphase region. A distinction is thus made between physical column sections (as determined by feed and drawoff streams) and the collocation modules, with sections that contain phase discontinuities being represented by the corresponding number of modules. The adjustable module lengths are treated as continuous variables with their sum constrained to be consistent with the physical dimensions of the column. The collocation treatment of an individual module (finite element) is first described. Thereafter, the module boundary equations and a solution procedure are discussed.

Collocation Treatment of a Multistage Module

The collocation treatment of a module parallels that given by Stewart and coworkers (1985) and Swartz and Stewart (1986), hence is only briefly described here.

A general N-stage module with P liquid phases is illustrated in Figure 2. The liquid component flows, vapor component flows, and enthalpies are approximated by polynomials using $n \le N$ interior grid points, together with the entry points: $s = 0$ for the liquid phases and $s = N + 1$ for the vapor. This gives the approximating functions

$$\underline{\tilde{\ell}}^{\alpha}(s) = \sum_{j=0}^{n} W_{\ell j}(s)\, \underline{\tilde{\ell}}^{\alpha}(s_j) \qquad 0 \le s \le N$$

$$\alpha = \mathrm{I}, \mathrm{II}, \ldots, P \tag{8}$$

$$\underline{\tilde{v}}(s) = \sum_{j=1}^{n+1} W_{vj}(s)\underline{\tilde{v}}(s_j) \qquad 1 \le s \le N+1 \tag{9}$$

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

$$\alpha = \mathrm{I}, \mathrm{II}, \ldots, P \tag{10}$$

$$\tilde{V}(s)\tilde{H}(s) = \sum_{j=1}^{n+1} W_{vj}(s)\tilde{V}(s_j)\tilde{H}(s_j) \qquad 1 \le s \le N+1 \tag{11}$$

in which

$$\tilde{L}^{\alpha}(s) = \sum_{i=1}^{c} \tilde{\ell}_i^{\alpha}(s) \qquad \alpha = \mathrm{I}, \mathrm{II}, \ldots, P$$

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

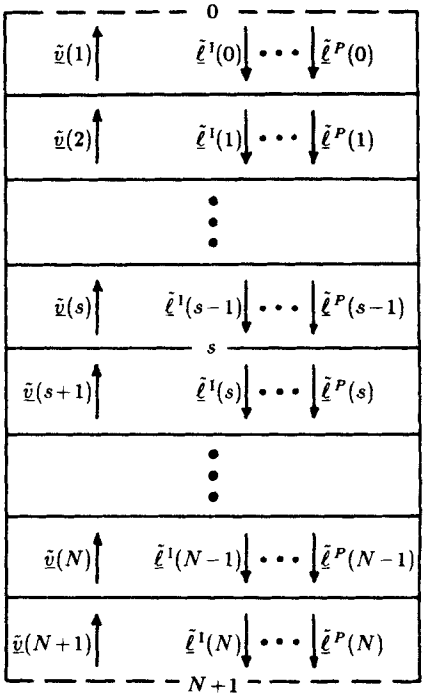

Figure 2. Multistage module with P liquid phases.

The W functions in Eq. 8–11 are Lagrange polynomials, given by

$$W_{kj}(s) = \prod_{\substack{k=0 \\ k \neq j}}^{n} \frac{(s - s_k)}{(s_j - s_k)} \qquad j = 0, \ldots, n \tag{12}$$

$$W_{vj}(s) = \prod_{\substack{k=1 \\ k \neq j}}^{n+1} \frac{(s - s_k)}{(s_j - s_k)} \qquad j = 1, \ldots, n+1 \tag{13}$$

The tilde ($\sim$) denotes an approximating function.

Substitution of the approximating functions into the set of singe-stage MESH equations yields a corresponding set of residual functions continuous in s. The collocation equations are obtained by setting the residuals to zero at n interior grid points $s_1, \ldots, s_n$. The resulting equations, written in terms of component flows, are:

$$\sum_{\alpha=1}^{P} \underline{\tilde{\ell}}^{\alpha}(s_j - 1) + \underline{\tilde{v}}(s_j + 1) - \sum_{\alpha=1}^{P} \underline{\tilde{\ell}}^{\alpha}(s_j) - \underline{\tilde{v}}(s_j) = \underline{0} \qquad j = 1, \ldots, n \tag{14}$$

$$\underline{\tilde{y}}(s_j) - \underline{\tilde{y}}(s_j + 1) - \underline{\underline{\tilde{E}}}^{\alpha}_{MV}(s_j)\,[\underline{y}^{*}[\underline{\tilde{x}}^{\alpha}(s_j), \tilde{T}(s_j), \tilde{p}(s_j)] - \underline{\tilde{y}}(s_j + 1)] = \underline{0} \qquad j = 1, \ldots, n \qquad \alpha = \mathrm{I}, \mathrm{II}, \ldots, P \tag{15}$$

where

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

$$\underline{\tilde{x}}^{\alpha}(s) = \frac{\tilde{\ell}^{\alpha}(s)}{\tilde{L}^{\alpha}(s)} \qquad \alpha = \mathrm{I}, \mathrm{II}, \ldots, P$$

$$\sum_{\alpha=1}^{P} \tilde{L}^{\alpha}(s_j - 1)\tilde{h}^{\alpha}(s_j - 1) + \tilde{V}(s_j + 1)\tilde{H}(s_j + 1) - \sum_{\alpha=1}^{P} \tilde{L}^{\alpha}(s_j)\tilde{h}^{\alpha}(s_j) - \tilde{V}(s_j)\tilde{H}(s_j) = 0 \qquad j = 1, \ldots, n \tag{16}$$

The collocation points $s_1, \ldots, s_n$ in a given module are calculated as the zeros of the Hahn polynomial $Q_n(s - 1; 0, 0, N - 1)$. A detailed discussion of this choice of collocation points, including formulas for calculating them, is given by Stewart et al. (1985). These zeros are readily computable for any real number $N \geq n$, as explained by Swartz and Stewart (1986).

Equations 14–16 may also be used to describe an equilibrium condenser and an equilibrium reboiler by including a condenser heat duty Q_C and a reboiler heat duty Q_R in the respective balance equations, and equating the extraneous flows to zero.

The modular analysis of a complete distillation system is easy when the number of phases is uniform throughout the system. The linkages between the modules are expressed by simple material and energy balances.

A two-phase system of M modules, for example, is then described by $\Sigma_{k=1}^{M} n^{(k)}(2c + 1)$ collocation equations and $M(2c + 2)$ module linkage equations, where $n^{(k)}$ denotes the number of collocation points in module k. The unknowns are the component flows and temperatures at the interior grid points, and the component flows and stream enthalpies at the entry points. The Murphree vapor efficiencies, column pressure, and condenser and reboiler heat duties are assumed here to be specified. In practice, the working equation system can be condensed significantly by direct elimination of the module entrance variables.

Module Boundary Location as a Variable

The boundaries of the multiphase regions are now considered. By definition, these locations are such that the additional liquid phase is just beginning to form (or has just disappeared) according to our interpolation of states along the column length. We accordingly require the newly forming or vanishing liquid phase at the boundary to be in equilibrium with the other liquid phases at that location, and to be infinitesimal in amount. This is analogous to a bubble-point condition.

Consider first the case in which a new phase appears, as illustrated in Figure 3a. For illustration, the upper module, k, is assumed to contain a single liquid phase. Parenthesized superscripts are used to denote the corresponding modules. The above criteria for the boundary location give the algebraic equations:

$$[\underline{\tilde{\ell}}^{\mathrm{I}}(s_0)]^{(k+1)} = [\underline{\tilde{\ell}}(N)]^{(k)} \tag{17}$$

$$[\underline{\tilde{\ell}}^{\mathrm{II}}(s_0)]^{(k+1)} = \underline{0} \tag{18}$$

$$\gamma_i^{\mathrm{I}}[\tilde{x}_i^{\mathrm{I}}(s_0)]^{(k+1)} = \gamma_i'' x_i'' \qquad i = 1, \ldots, c \tag{19}$$

$$\sum_{i=1}^{c} x_i'' = 1 \tag{20}$$

with

$$[\underline{\tilde{x}}^{\mathrm{I}}(s_0)]^{(k+1)} = \frac{[\underline{\tilde{\ell}}^{\mathrm{I}}(s_0)]^{(k+1)}}{[\tilde{L}^{\mathrm{I}}(s_0)]^{(k+1)}}. \tag{21}$$

Here γ_i^{I} and γ_i'' are activity coefficients given as functions of composition and temperature.

The liquid enthalpy entrance equations for module $k + 1$ follow immediately:

$$[\tilde{L}^{\mathrm{I}}(s_0)]^{(k+1)}[\tilde{h}^{\mathrm{I}}(s_0)]^{(k+1)} = [\tilde{L}(N)]^{(k)}[\tilde{h}(N)]^{(k)} \tag{22}$$

$$[\tilde{L}^{\mathrm{II}}(s_0)]^{(k+1)}[\tilde{h}^{\mathrm{II}}(s_0)]^{(k+1)} = 0 \tag{23}$$

By making the interpolated vapor functions continuous at the boundary, one obtains the following vapor entrance equations for module k:

$$[\underline{\tilde{v}}(s_{n+1})]^{(k)} = [\underline{\tilde{v}}(1)]^{(k+1)} \tag{24}$$

$$[\tilde{V}(s_{n+1})]^{(k)}[\tilde{H}(s_{n+1})]^{(k)} = [\tilde{V}(1)]^{(k+1)}[\tilde{H}(1)]^{(k+1)} \tag{25}$$

Thus, the material and energy balance equations for linkage of the two modules are augmented by Eqs. 19 and 20. The corresponding $c + 1$ additional variables are the compositions $\underline{x}''$ and the module length $N^{(k)}$. The length of the remainder of the section is obtained by subtracting $N^{(k)}$ from the total number of stages in the given column section.

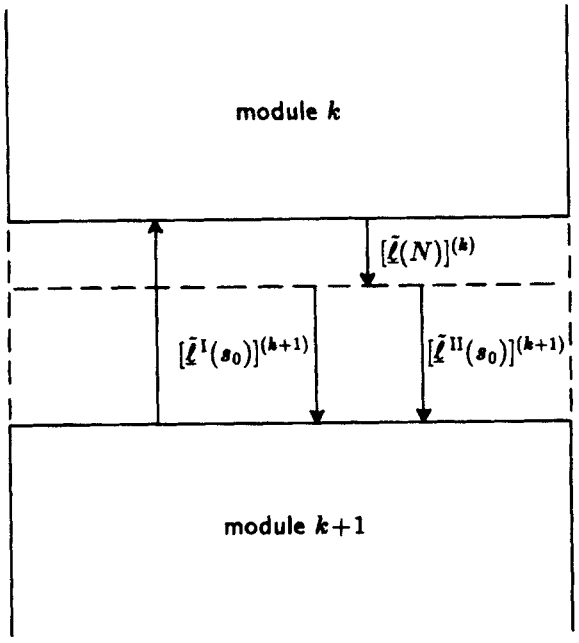

Figure 3a. Module boundary arrangement for formation of a second liquid phase.

The case in which the second liquid phase disappears, as illustrated in Figure 3b, can be treated analogously. Here, the two liquid phases leaving the upper module combine to form a single phase. The corresponding boundary equations are

$$[\tilde{\underline{\ell}}(s_0)]^{(k+1)} = [\tilde{\underline{\ell}}^{I}(N)]^{(k)} + [\tilde{\underline{\ell}}^{II}(N)]^{(k)} \tag{26}$$

$$\gamma_i[\tilde{x}_i(s_0)]^{(k+1)} = \gamma_i'' x_i'' \quad i = 1, \ldots, c \tag{27}$$

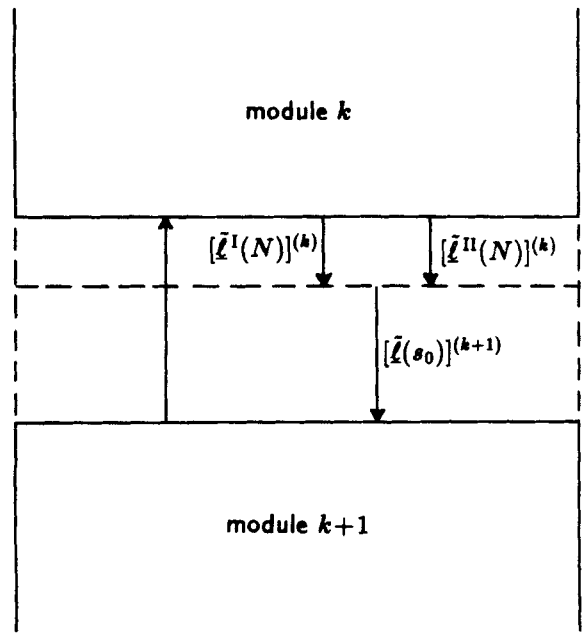

Figure 3b. Module boundary arrangement for disappearance of a second liquid phase.

$$\sum_{i=1}^{c} x_i'' = 1 \tag{28}$$

in which

$$[\tilde{\underline{x}}(s_0)]^{(k+1)} = \frac{[\tilde{\underline{\ell}}(s_0)]^{(k+1)}}{[\tilde{L}(s_0)]^{(k+1)}}. \tag{29}$$

The energy balance

$$[\tilde{L}(s_0)]^{(k+1)}[\tilde{h}(s_0)]^{(k+1)} = [\tilde{L}^{I}(N)]^{(k)}[\tilde{h}^{I}(N)]^{(k)} + [\tilde{L}^{II}(N)]^{(k)}[\tilde{h}^{II}(N)]^{(k)} \tag{30}$$

completes the set of liquid entrance equations.

The vapor boundary equations are again given by Eqs. 24 and 25. As before, there are $c + 1$ additional equations and variables associated with the calculation of the module boundary location.

Solution Procedure

The initial distribution of breakpoints was obtained by calculating first a two-phase solution (possibly degenerate), followed by stability tests on the liquid phase at the collocation points and at the liquid entrance and exit positions for each module. The phase stability algorithm given by Fournier and Boston (1981) was used in the latter calculations. Column sections containing phase discontinuities were then subdivided into the indicated modules. Guesses for the states at the new collocation point locations were obtained by interpolation. The multiphase system of model equations was then solved by a damped Newton method, with each adjustable module length bounded from below by the corresponding number of collocation points.

In the discussion of the module equations, the condenser and reboiler heat duties were assumed to be specified. However, alternate specifications such as a given distillate flow rate and reflux ratio are easily accommodated. With unspecified condenser and reboiler heat duties, the number of system unknowns is increased by two. A given reflux ratio and distillate flow rate provide the following additional equations,

$$\sum_{i=1}^{c} \tilde{v}_{C,i} = D \tag{31}$$

$$\sum_{i=1}^{c} \tilde{\ell}_{C,i} = R\left(\sum_{i=1}^{c} \tilde{v}_{C,i}\right) \tag{32}$$

where D and R are the specified distillate flow rate and reflux ratio, respectively. These alternate specifications were used in the example problems.

Example Problems

The first problem studied here was considered originally by Block and Hegner (1976), and later by Ross and Seider (1981) and Buzzi Ferraris and Morbidelli (1981, 1982). The system consists of a 10-tray propanol-butanol-water fractionator, with the feed introduced as liquid on the fourth tray. The problem specifications are listed in Table 1. The thermodynamic data of Buzzi Ferraris and Morbidelli (1981) were used.

The preliminary two-phase solution to problem 1 was calculated using two collocation points in each of the rectifying and

Table 1. Test Problem Specifications

	Problem No.	
	1	2
No. components	3	3
No. rectifying stages	3	10
No. stripping stages	7	6
Feed composition, mol frac.	Butanol (1): 0.13 Water (2): 0.65 Propanol (3): 0.22	Acrylonitrile (1): 0.40 Acetonitrile (2): 0.35 Water (3): 0.25
Total feed, kmol/h	50	100
Feed temp., K	363.0	344.8
Stage efficiencies	1.0	1.0
Condenser type	Equilibrium	Equilibrium
Reboiler type	Equilibrium	Equilibrium
Pressure, MPa	0.1013	0.1013
Distillate rate, kmol/h	29.0	60.8
Reflux ratio	3.5	21.71

Table 2. Comparison of Solutions to Problem 1: Condenser States

Method	Stream	Mol Frac. (1)	(2)	(3)	Total Flow, kmol/h	Temp., K
Collocation	V	0.0263	0.6204	0.3534	29.00	362.17
	L	0.0502	0.6450	0.3048	101.50	
Full-order	V	0.0262	0.6203	0.3534	29.00	362.17
	L	0.0502	0.6450	0.3048	101.50	

Table 3. Comparison of Solutions to Problem 1: Reboiler States

Method	Stream	Mol Frac. (1)	(2)	(3)	Total Flow, kmol/h	Temp., K
Collocation	V	0.2052	0.7536	0.0412	135.90	365.91
	L^{I}	0.2999	0.6612	0.0389	19.00	
	L^{II}	0.0212	0.9725	0.0064	2.00	
Full-order	V	0.2053	0.7536	0.0411	135.90	365.91
	L^{I}	0.2999	0.6612	0.0389	18.99	
	L^{II}	0.0212	0.9725	0.0064	2.01	

stripping sections. The stripping section was then subdivided into two modules in accordance with results of the phase stability test, and the resulting system was analyzed with two collocation points in each of the three multistage modules. A full-order solution was also computed against which the approximate solution could be compared. Results of the two solution procedures are given in Tables 2 and 3 and in Figures 4 to 6. The limiting values of the mole fractions at the inlet of the two-liquid phase module were calculated using L'Hospital's rule. The collocation solution is seen to agree closely with that obtained using the full stagewise model.

Our second problem involves the acrylonitrile-acetonitrile-water system studied by Buzzi Ferraris and Morbidelli (1982). The separation is carried out in a 16-tray column with the feed introduced on the eleventh tray. The complete problem specifications are listed in Table 1. The thermodynamic data of the above-cited workers were used.

Problem 2 was solved initially as a two-phase problem with three collocation points in the rectifying section and two collocation points in the stripping section. The phase stability test indi-

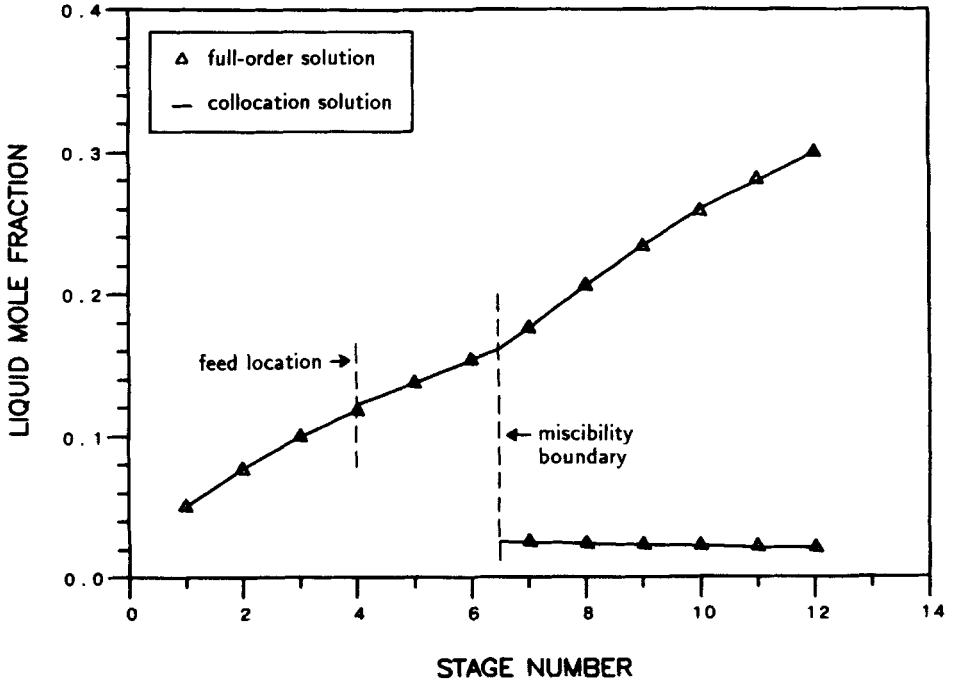

Figure 4. Results for butanol liquid mole fraction in problem 1.

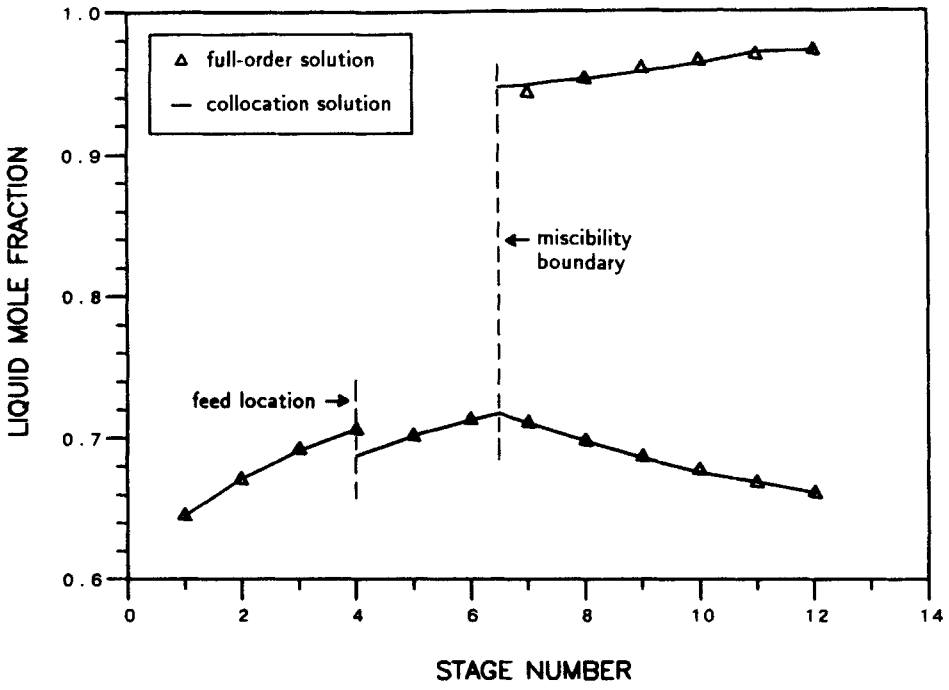

Figure 5. Results for water liquid mole fraction in problem 1.

cated a change in the number of phases in the rectifying section. The resulting three-phase problem was solved with two collocation points in each of the three multistage modules. Tables 4 and 5 provide a comparison of the collocation and full-order results for the condenser and reboiler. Comparisons of the liquid mole fraction profiles are given in Figures 7 to 9. The mole fractions $\underline{x}''$ described in Eqs. 27 and 28 were used as limiting values for the second liquid phase in Figures 7–9. L'Hospital's rule is not useful in this case, since the outlet component flows for phase II evaluated via Eq. 8 would not in general vanish identically. The collocation results are seen to be excellent.

Discussion

In this finite-element approach the boundaries of the multiphase regions are computed to achieve thermodynamic stability

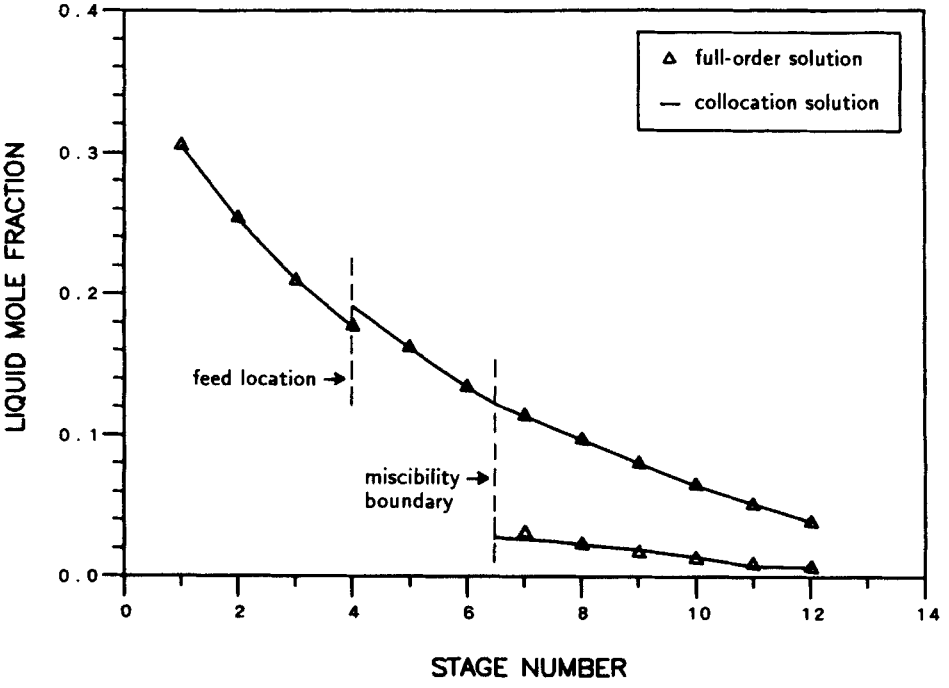

Figure 6. Results for propanol liquid mole fraction in problem 1.

Table 4. Comparison of Solutions to Problem 2: Condenser States

Method	Stream	Mol Frac. (1)	(2)	(3)	Total Flow, kmol/h	Temp., K
Collocation	V	0.6362	0.0667	0.2971	60.80	343.57
	L^{I}	0.6206	0.0935	0.2859	1,292.64	
	L^{II}	0.0538	0.0183	0.9279	27.33	
Full-order	V	0.6363	0.0666	0.2971	60.80	343.57
	L^{I}	0.6207	0.0934	0.2859	1,291.48	
	L^{II}	0.0538	0.0182	0.9279	28.49	

Table 5. Comparison of Solutions to Problem 2: Reboiler States

Method	Stream	Mol Frac. (1)	(2)	(3)	Total Flow, kmol/h	Temp., K
Collocation	V	0.0397	0.7068	0.2535	1,353.52	350.06
	L	0.0337	0.7894	0.1769	39.20	
Full-order	V	0.0396	0.7069	0.2535	1,353.81	350.06
	L	0.0335	0.7895	0.1769	39.20	

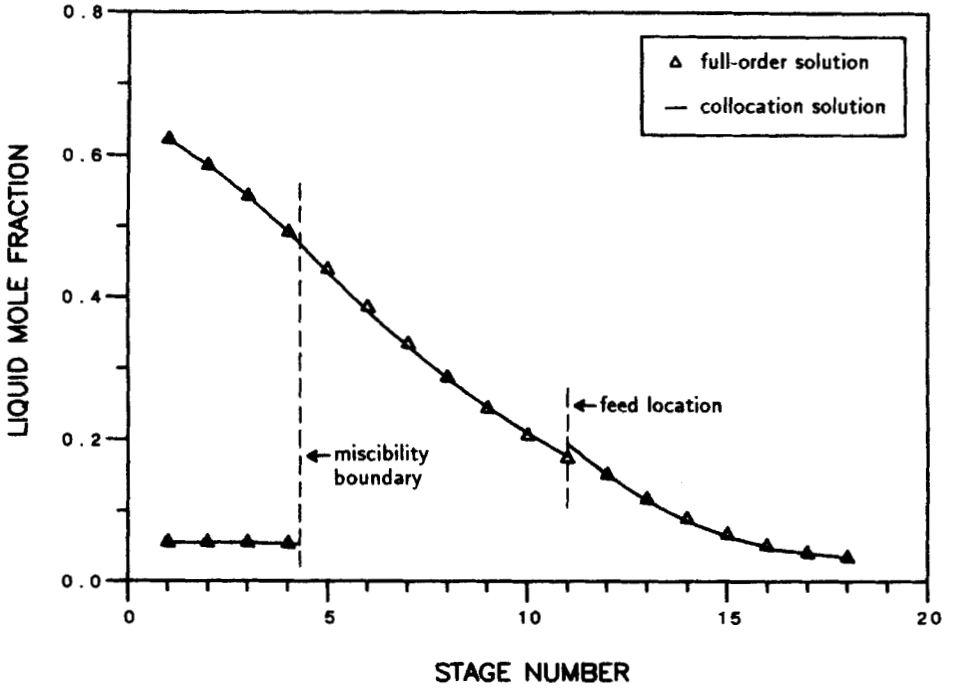

Figure 7. Results for acrylonitrile liquid mole fraction in problem 2.

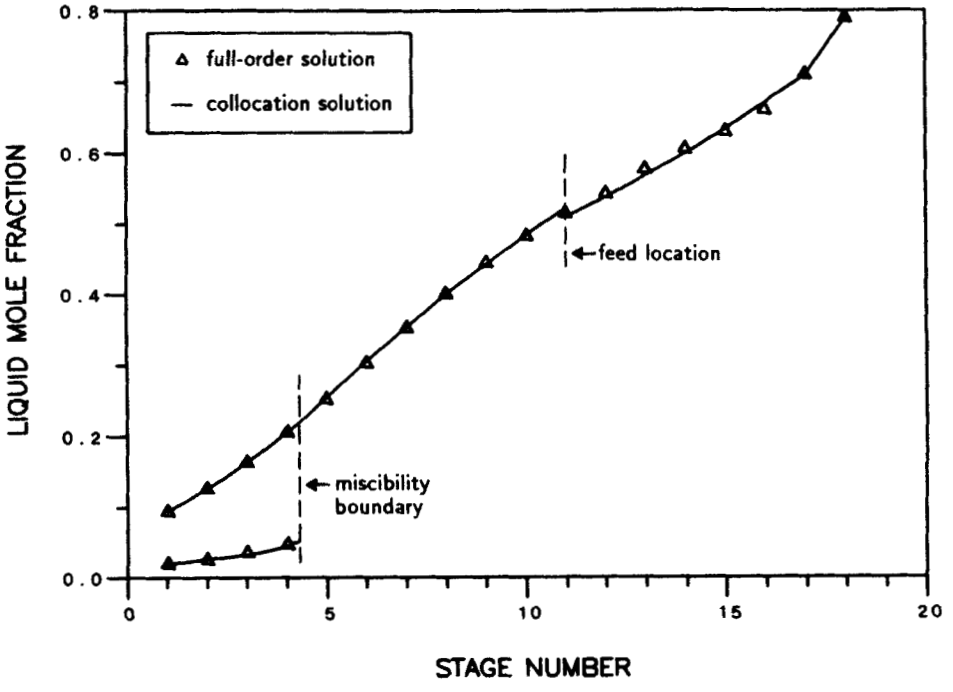

Figure 8. Results for acetonitrile liquid mole fraction in problem 2.

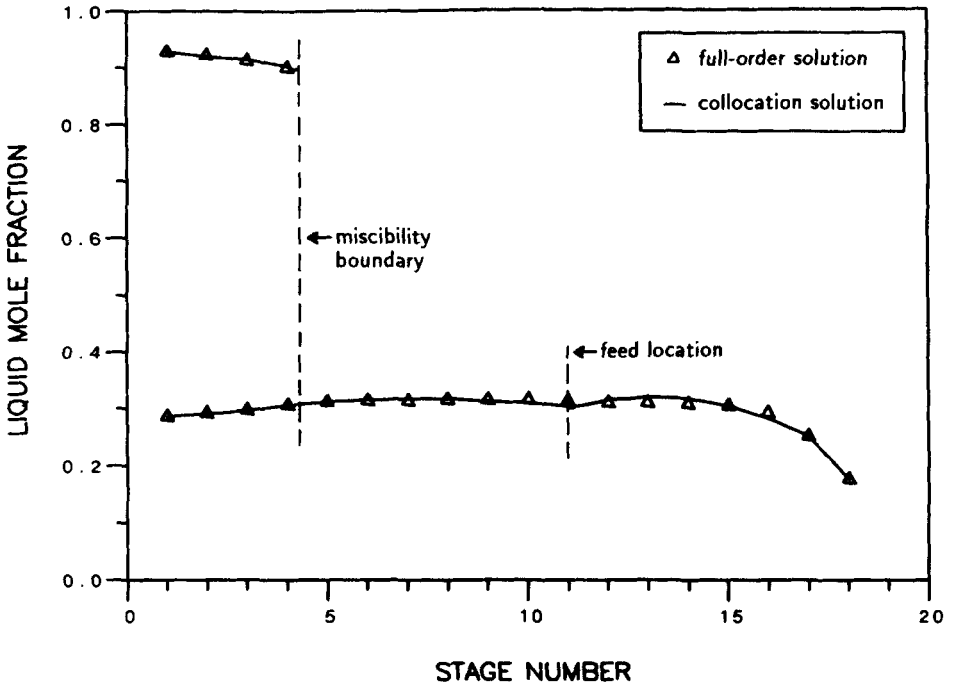

Figure 9. Results for water liquid mole fraction in problem 2.

of the interpolated total liquid streams. The boundary locations are included directly as variables in the collocation equations. The initial allocation of the multiphase modules is done by first solving the system as a two-phase problem, then testing the stability of the liquid phase at the collocation points and liquid entrance and exit positions of each module. The module boundary locations are updated simultaneously with the other system variables during the Newton iteration, rather than in an additional outer iteration loop as in prior methods based on the full stagewise model. Phase stability testing could also be performed on the converged finite-element solution as a final check on the phase pattern; this proved unnecessary in the examples presented here.

Solution of the full system of equations by Newton's method provides great flexibility with regard to allowable specifications (subject to the requirement of a well-posed problem). The proposed collocation method is readily applied to distillation design, following the approach given by Swartz and Stewart (1986). In that case, the section lengths would be included as variables in an optimization calculation.

Acknowledgment

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Notation

c = number of components
D = distillate molar flow rate, kmol/h
$\underline{\underline{E}}_{MV}$ = Murphree vapor efficiency matrix
h = liquid molar enthalpy, kJ/kmol
H = vapor molar enthalpy, kJ/kmol
$\underline{\ell}$ = vector of liquid component flows, kmol/h
$\underline{\ell}_C$ = vector of liquid component flows from condenser, kmol/h
L = liquid molar flow rate, kmol/h
M = number of modules
n = degree of polynomial; number of collocation points in module
N = module length, stages
p = pressure at mass transfer interface
P = number of liquid phases
Q_C = condenser heat duty, kJ/h
Q_R = reboiler heat duty, kJ/h
R = reflux ratio
s = stage coordinate
s_j = jth collocation point
T = temperature, K
$\underline{v}$ = vector of vapor component flows, kmol/h
$\underline{v}_C$ = vector of vapor component flows from condenser, kmol/h
V = vapor molar flow rate, kmol/h
$W_{\ell j}(s)$ = Lagrange polynomial for liquid states
$W_{vj}(s)$ = Lagrange polynomial for vapor states
$\underline{x}$ = liquid mole fraction vector
$\underline{y}$ = vapor mole fraction vector
$\underline{y}^*(\underline{x}, T, p)$ = vapor bubble-point composition corresponding to liquid state $(\underline{x}, T, p)$

Greek symbols

γ = activity coefficient

Subscripts

i = ith component
s = stage s

Superscripts

α = liquid phase α, where α may take on values I, II, . . . , P
$''$ = equilibrium state of newly forming or vanishing liquid phase
(k) = kth module

Abbreviations

MESH = Material balance equations, Efficiency relations, Summation equations, and energy (Heat) balance equations.

Operations

$\tilde{f}(s)$ = continuous approximation to stagewise function f_s

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