NONLINEAR BOUNDARY VALUE PROBLEMS AND MULTICOMPONENT DISTILLATION

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Abstract—Multicomponent distillation is essentially a nonlinear boundary value problem in difference equations. Different computational approaches can be developed based on the choice of different parameters as the unknown variables, different stages as the initial stage, and different methods to solve the difference equations. In this work, these different aspects are explored. One particular interesting approach is to choose the $(m - 1)$ liquid phase concentrations and total liquid molal rate as the unknowns, where m is the number of components in the system. This approach results in a system of nonlinear simultaneous mixed difference and algebraic equations and presents some interesting computational problems.

1. INTRODUCTION

In an earlier paper Noh and Lee (1971), the quasilinearization technique was used to solve multicomponent distillation problems. We wish to show in this work that the concept of treating multicomponent distillation as nonlinear boundary value problems in difference equations is a powerful approach. Many different algorithms can be formulated by the combined use of this concept and quasilinearization. For example, the computation of the multistage process can commence at any stage in the column as long as appropriate boundary conditions are used. Three different starting points, namely the condenser, the reboiler, and the feed stage are illustrated in this paper.

A second aspect concerns the choice of unknown variables. In the earlier paper (Noh and Lee, 1971) the liquid phase concentration was used as the unknown variables. Any other parameters such as vapor phase concentration, total flow rate of the vapor or liquid, temperature, and the flow rates of the individual components can also be used as the unknown variables provided that the number of unknown variables is equal to the number of components in the system. To illustrate this concept, $(m - 1)$ liquid phase concentrations plus total liquid phase flow rate will be used as the unknown variables in this work. The number m represents the number of components in the system. This approach results in a system of simultaneous mixed difference and algebraic equations and presents some interesting computation problems. In a latter paper, the use of $(m - 1)$ liquid phase concentrations plus temperature as unknown variables will be discussed.

A third aspect concerns the direction of computation. It is shown in this work that the computation can be carried out in any one direction or in any mixed directions.

2. FEED STAGE AS THE INITIAL STAGE AND LIQUID PHASE COMPOSITION AS THE UNKNOWN VARIABLES

The basic equations for a multicomponent distillation column with liquid phase mole fractions as the unknown variables have been obtained in an earlier paper (Noh and Lee, 1971) by using conventional material and enthalpy balances and by eliminating all the unknown parameters except liquid phase compositions. The resulting equations for a system with a total condenser are

$$g_i(n) = [k_i(n + 1)x_i(n + 1) - x_i(0)] \sum_{j=1}^{m} x_j(n)h_j(n)$$

$$+ [x_i(0) - x_i(n)] \sum_{j=1}^{m} k_j(n + 1)x_j(n + 1)H_j(n + 1)$$

$$+ [x_i(n) - k_i(n + 1)x_i(n + 1)]\left[\frac{Q_c}{D} + \sum_{j=1}^{m} x_j(0)h_j(0)\right] = 0 \qquad n = 1, 2, \ldots, f - 1. \quad (1)$$

$$g_i(n) = \left[k_i(n+1)x_i(n+1) - \frac{F}{B}x_{if} + \frac{D}{B}x_i(0) \right] \sum_{j=1}^{m} x_j(n)h_j(n)$$

$$+ \left[\frac{F}{B}x_{if} - \frac{D}{B}x_i(0) - x_i(n) \right] \sum_{j=1}^{m} k_j(n+1)x_j(n+1)H_j(n+1)$$

$$+ [x_i(n) - k_i(n+1)x_i(n+1)] \frac{1}{B} \left[F \sum_{j=1}^{m} x_{if}h_{if} \right.$$

$$\left. - D \sum_{j=1}^{m} x_j(0)h_j(0) - Q_c \right] = 0 \qquad n = f, f+1, \ldots, N, \tag{2}$$

with $i = 1, 2, \ldots, m$, where m is the number of components in the system, $x_i(n)$ denotes the mole fraction of component i leaving plate n in the liquid phase, F, D, and B denote the total molal rates of the feed, distillate, and bottom streams, respectively, k_i, h_i, and H_i denote the equilibrium constant, liquid phase enthalpy, and vapor phase enthalpy of the ith component, respectively, and f denotes the feed stage. The plates are numbered consecutively down from the top of the column to the reboiler. The condenser is assigned the number zero, and the boiler the number $(N+1)$. The subscripts f and c denote the feed stream and the condenser, respectively. An expression for the condenser duty Q_c can be obtained by using enthalpy balance around the condenser. For a total condenser, Q_c can be represented by

$$Q_c = V(1) \sum_{j=1}^{m} x_j(0)[H_j(1) - h_j(0)]. \tag{3}$$

For a total condenser, the zeroth stage or condenser can be represented by

$$x_i(0) = k_i(1)x_i(1), \qquad i = 1, 2, \ldots, m, \tag{4}$$

where $V(1)$ is the total molal flow rate leaving plate one in the vapor phase.

Following the Thiele and Geddes assumptions, we shall assume that the following quantities are specified: the flow rate, thermal condition and composition of the feed, the number of plates, feed plate location, column pressure, and two other variables. These two other variables can be any two of the three variables, D, $L(0)$, and $V(1)$, where $L(0)$ represents the total molal flow rate leaving the condenser at the liquid phase. Noting that when any two of the three variables are specified, the third one can be obtained by using the total material balance equation around the condenser.

Equations (1), (2) and (4) represent m first order nonlinear difference equations over the entire column including both the condenser and the reboiler. The m unknowns are $x_i(n)$, $i = 1, 2, \ldots, m$. The parameters k, h, and H are functions of the temperature T. The temperature, in turn, is a function of the liquid phase composition through the bubble point temperature equation

$$\sum_{j=1}^{m} k_j(n)x_j(n) = 1, \tag{5}$$

for all n. Thus, k, h and H are not unknowns but are implicit functions of $x_i(n)$ through T. All the other quantities in equations (1)–(4) are given. Notice that B can be obtained easily once D and F are given.

The boundary conditions for this system of first order difference equations are

$$Fx_{if} = Dx_i(0) + Bx_i(N+1), \qquad i = 1, 2, \ldots, m. \tag{6}$$

In an earlier paper (Noh and Lee, 1971) the above mixed boundary value problem was solved by quasilinearization and by commence the computation at $n = 0$. We wish to solve the same problem by quasilinearization except that the feed stage, or $n = f$, is treated as the initial stage. Equations (1) and (2) can be represented symbolically by the vector equation

$$g(x(0), x(n), x(n+1)) = 0, \qquad n = 1, 2, \ldots, N, \tag{7}$$

where g and x are m dimensional vectors and the three x vectors are the unknowns in equations (1) and (2). The above equation can be linearized as (Noh and Lee, 1971; Bellman and Kalaba, 1965; Lee, 1968)

$$g_k + J_{x(n)}[x_{k+1}(n) - x_k(n)] + J_{x(n+1)}[x_{k+1}(n+1) - x_k(n+1)], \tag{8}$$

where the variables with subscript k are known variables and are obtained during the previous kth iteration. The matrix J is Jacobian matrix and is functions of the kth iteration variables.

We have omitted $x_i(0)$ in equations (1) and (2) in the above linearization. In actual computation, the results for $x_i(0)$ of the previous kth iteration will be used in the current $(k + 1)$st iteration. Since our computation commence at the feed stage, the values of $x_i(0)$ are unknown values until the end of the computation. The elements of the Jacobian matrix can be obtained by partial differentiation. For example, the elements of $J_{x(n)}$ can be obtained by partial differentiation of equations (1) and (2) with respect to $x(n)$. Due to the presence of h and H, implicit differentiations must be used. The resulting expressions are fairly complicated and they will not be listed here. However, this procedure for obtaining the implicit differentiations using equation (5) has been discussed in an earlier paper (Noh and Lee, 1971). For example, the elements for $J_{x(n+1)}$ for the rectifying section can be represented by

$$\frac{\partial g_i(n)}{\partial x_j(n+1)} = \left[\sum_{r=1}^{m} x_r(n)h_r(n) - \frac{Q_c}{D} - \sum_{r=1}^{m} x_r(0)h_r(0) \right] k_i(n+1)\delta_{ij} + [x_i(0) - x_i(n)] \left[k_j(n+1)H_j(n+1) \right.$$

$$\left. - \sum_{r=1}^{m} k_r(n+1)x_r(n+1)H'_r(n+1) \frac{k_j(n+1)}{\sum_{r=1}^{m} x_r(n+1)k'_r(n+1)} \right] \quad i, j = 1, 2, \ldots, m, \tag{9}$$

with $n = 1, 2, \ldots, f - 1$, where

$$\delta_{ij} = 0, \quad i \neq j$$
$$= 1, \quad i = j$$

and

$$H' = \frac{dH}{dT}, \quad k' = \frac{dk}{dT},$$

where we have omitted the subscript k on all the variables.

In addition to $x_i(0)$, the functions $k_i(n + 1)$ and $H_j(1)$ are also not considered in linearization. Strictly speaking and also to obtain the quadratic convergence property of quasilinearization, all nonlinear functions should be linearized. However, practical experience indicates that due to the implicit differentiation, if $k_i(n + 1)$ is also considered for linearization, the resulting linear equations are so complicated that unreasonably large or small values are obtained for the particular and homogeneous solutions. Since $H_j(1)$ appears only in equation (3), practical experience indicates that the linearization of the function $H_j(1)$ does not influence the convergence rate to any noticeable degree.

The general solution for the linearized equation (6) can be represented by

$$x_{i,k+1}(n) = x_{ip,k+1}(n) + \sum_{j=1}^{m} a_j x_{ihj,k+1}(n) \tag{10}$$

$$i = 1, 2, \ldots, m_j \qquad n = 0, 1, 2, \ldots, N + 1,$$

where a represents the integration constants, the subscripts h and p represent the homogeneous and particular solutions, respectively. These particular and homogeneous solutions can be obtained by solving the linearized equations with assumed initial conditions at the feed stage. For the rectifying section, the computation is carried out from the feed stage upward until the condenser. For the stripping section, this computation is carried out from the feed stage downward until the reboiler. Any reasonable values can be used for the initial conditions as long as the initial conditions used for the homogeneous solutions are nontrivial and distinct.

Once the particular and m sets of homogeneous solutions are obtained, the integration constants can be calculated by substituting equation (10) into the boundary condition equation (6). The resulting equations represent a system of algebraic equations with a's as the only unknowns. After obtaining the values of a, the general solution can be obtained by using equation. Call this just obtained general solution as the kth iteration, $(k + 1)$st can be calculated in a similar manner. This iterative procedure is continued until the desired accuracy is obtained. A detailed discussion of the computational procedure is given, see ref. Lee, 1968.

Numerical results

The same problem solved by Noh and Lee (1971) and originally solved by Holland (1963) is solved. The problem has five hydrocarbon components. The numerical values used are

$$x_{1f} = 0.05, \ x_{2f} = 0.15, \ x_{3f} = 0.25$$
$$x_{4f} = 0.20, \ x_{5f} = 0.35, \ N = 9 \tag{11}$$
$$f = 5, \ F = 100, \ D = 48.9, \ v(1) = 175.$$

The feed is boiling point liquid and a total condenser is used. The functions H, h, and k have been correlated as functions of temperature by Holland (1963). The initial conditions used to obtain the homogeneous and particular solutions are listed in Table 1. To start the iteration, the feed composition is used as the initial approximation, or

$$x_{1,k=0}(n) = 0.05, \ x_{2,k=0}(n) = 0.15, \ x_{3,k=0}(n) = 0.25$$
$$x_{4,k=0}(n) = 0.20, \ x_{5,k=0}(n) = 0.35, \tag{12}$$

for all n. The convergence rates of the distillate composition and distillate rate are shown in Table 2. As can be seen that the convergence rate is slower than that obtained in an earlier paper (Noh and Lee, 1971). This is caused by the fact that $x_i(0)$, $i = 1, 2, \ldots, m$, was not considered in linearization. This difficulty can be avoided it in making the material balance, the condenser stage is not always included and hence $x_i(0)$ does not appear in equations (1) and (2).

Table 1. Initial conditions used for obtaining particular and homogeneous solutions using feed as the initial stage

Variable	Particular solution	Homogeneous solution				
		1	2	3	4	5
$x_1(5)$	0.2	0.3	0.2	0.2	0.2	0.1
$x_2(5)$	0.2	0.2	0.3	0.2	0.2	0.2
$x_3(5)$	0.2	0.2	0.2	0.3	0.2	0.2
$x_4(5)$	0.2	0.2	0.2	0.2	0.3	0.2
$x_5(5)$	0.2	0.1	0.1	0.1	0.1	0.3

Table 2. Convergence rates of distillate composition and distillate rate using feed as the initial stage

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$x_5(0)$	D
0	0.05	0.15	0.25	0.20	0.35	—
1	0.1108	0.3767	0.5965	−0.1211	−0.1748	38.54
2	0.1022	0.2767	0.3854	0.2261	0.1454	55.54
3	0.1031	0.3013	0.4685	−0.0153	−0.0009	41.89
4	0.0999	0.2749	0.4093	0.1273	0.0789	48.43
5	0.1010	0.2909	0.4526	0.0358	0.0294	44.49
6	0.1011	0.2890	0.4419	0.0764	0.0483	46.78
7	0.1012	0.2922	0.4535	0.0511	0.0366	45.70
8	0.1015	0.2934	0.4555	0.0661	0.0456	47.04
9	0.1015	0.2942	0.4584	0.0584	0.0418	46.67
10	0.1017	0.2958	0.4616	0.0652	0.0462	47.46
15	0.1020	0.2981	0.4677	0.0682	0.0494	48.18
20	0.1021	0.2994	0.4709	0.0708	0.0517	48.65
25	0.1022	0.2997	0.4716	0.0719	0.0525	48.80
30	0.1022	0.2999	0.4721	0.0722	0.0528	48.86

3. REBOILER AS THE INITIAL STAGE AND LIQUID PHASE COMPOSITION AS THE UNKNOWN VARIABLES

Instead of used the condenser or the feed stage as the initial stage, the reboiler will be used as the initial stage in this section. Equations (1)–(7) remain unchanged. However, in order to increase the convergence rate, $k_i(n + 1)$ will also be considered in the linearization of equation (7). Equation (8) remains unchanged. But because of the linearization with respect to $k_i(n + 1)$, the Jacobians are different from those shown in equation (9). The elements for the Jacobian $J_{x(n+1)}$ for the rectifying Section are

$$\frac{\partial g_i(n)}{\partial x_j(n + 1)} = \left[\sum_{r=1}^{m} x_r(n)h_r(n) - \frac{Q_c}{D} - \sum_{r=1}^{m} x_r(0)h_r(0) \right]$$

$$\times \left[k_i(n + 1)\delta_{ij} - \frac{k_j(n + 1)}{\sum_{r=1}^{m} x_r(n + 1)k'_r(n + 1)} x_i(n + 1)k'_i(n + 1) \right]$$

$$+ [x_i(0) - x_i(n)]\left[k_j(n + 1)H_j(n + 1) \right.$$

$$- \left\{ \sum_{r=1}^{m} k_r(n + 1)x_r(n + 1)H'_j(n + 1) + \sum_{r=1}^{m} k'_r(n + 1)x_r(n + 1)H_r(n + 1) \right\}$$

$$\left. \times \frac{k_j(n + 1)}{\sum_{r=1}^{m} x_r(n + 1)k'_r(n + 1)} \right] \quad i,j = 1, 2, \ldots, m, \tag{13}$$

with $n = 1, 2, \ldots, f - 1$. Because of the linearization with respect to $x_i(n + 1)$, equation (13) is a much more complicated expression than equation (9). The elements of the other Jacobians can be obtained in a similar manner. Notice that $x_i(0)$ and $H_j(1)$ are still not considered in linearization.

Since $k_i(n)$ is considered in the linearization operation, equation (4) or the zeroth stage equation is no longer linear. This equation can be represented as

$$g_i(0) = x_i(0) - k_i(1)x_i(1) = 0, \quad i = 1, 2, \ldots, m. \tag{14}$$

Symbolically, this equation can be represented by the vector equation

$$g(x(0), x(1)) = 0, \tag{15}$$

which can be linearized as

$$g_k(0) + J_{x(0)}[x_{k+1}(0) - x_k(0)] + J_{x(1)}[x_{k+1}(1) - x_k(1)] = 0. \tag{16}$$

The elements of the Jacobian matrices can again be obtained by partial differentiation of equation (14). For $J_{x(0)}$, these elements are

$$\frac{\partial g_i(0)}{\partial x_j(0)} = \delta_{ij}, \quad i,j = 1, 2, \ldots, m. \tag{17}$$

The elements for $J_{x(1)}$ are

$$\frac{\partial g_i(0)}{\partial x_j(n)} = - k_i(1)\delta_{ij} + \frac{k_j(1)}{\sum_{r=1}^{m} x_r(1)k'_r(1)} k'_i(1)x_i(1), \quad i,j = 1, 2, \ldots, m. \tag{18}$$

Equation (10) remains the same. The computational procedure is essentially the same as before except that the initial conditions are given at $n = N + 1$ or the reboiler. The particular and homogeneous solutions are obtained by calculating upward commence at the reboiler. The initial

conditions at $n = N + 1$ are not listed. It should be emphasized that any reasonable sets of initial conditions can be used as long as the homogeneous solutions are nontrivial and distinct. Practical experience has indicated that the same general solution is obtained no matter what initial conditions are used as long as they satisfy the above specifications.

Using the numerical values listed in equation (11) and using the same initial approximations as those given in equation (12), the numerical results shown in Table 3 are obtained. As can be seen that since $k_i(n + 1)$ is also linearized, the convergence rate is much faster than that shown in Table 2. An even faster convergence rate can be obtained if $x_i(0)$ does not appear in equations (1) and (2). This can be achieved by performing the material balance from the reboiler instead of from the condenser of column. The resulting equations would include $x_i(N + 1)$ as unknowns in the difference equations. Thus, $x_i(N + 1)$ must be considered in the linearization.

Table 3. Convergence rates of distillate composition using reboiler as the initial stage

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$x_5(0)$
0	0.05	0.15	0.25	0.20	0.35
1	0.2072	0.8022	1.2772	−0.5207	−0.7659
2	0.1021	0.2761	0.5745	0.0330	0.0142
3	0.1022	0.3104	0.4502	0.0622	0.0749
4	0.1022	0.2976	0.4891	0.0794	0.0317
5	0.1022	0.3004	0.4624	0.0692	0.0657
10	0.1022	0.3001	0.4742	0.0725	0.0511
15	0.1022	0.3000	0.4719	0.0726	0.0533
19	0.1022	0.3000	0.4722	0.0726	0.0531

4. TOTAL LIQUID FLOW RATE AS AN UNKNOWN VARIABLE WITH BOUNDARY CONDITIONS AT FEED STATE

In the previous Sections, $x_i(n)$ was used as the m unknown variables and all the other parameters are considered as functions of $x_i(n)$. In practical designs, it is much more convenient if the m unknown variables are $(m - 1)x$'s and one liquid phase total molal rate. This choice of unknown variables results in a system of simultaneous mixed algebraic and difference equations. We shall show that this mixed system of equations can also be solved by the quasilinearization technique.

Eliminating the total molal vapor rate, $V(n + 1)$, and the mole fraction of component i in the vapor, $y_i(n + 1)$, from the four equations which are obtained by using the total material balance, individual material balance, enthalpy balance and the equilibrium ratio relationship, the following two equations can be obtained for the rectifying section

$$g_i(n) = [L(n) + D]k_i(n + 1)x_i(n + 1) - L(n)x_i(n) - Dx_i(0) = 0,$$
$$i = 1, 2, \ldots, m - 1; \quad n = 1, 2, \ldots, (f - 1) \tag{19a}$$

$$g_m(n) = [L(n) + D] \sum_{j=1}^{m} k_i(n + 1)H_j(n + 1)x_j(n + 1)$$
$$- L(n) \sum_{j=1}^{m} x_j(n)h_j(n) - D \sum_{j=1}^{m} x_j(0)h_j(0) - Q_c = 0 \qquad n = 1, 2, \ldots, (f - 1), \tag{20}$$

where the material and enthalpy balances were obtained by considering a section of the column which includes the condenser and any stage n. The flow rate $L(n)$ represents the total liquid phase molal rate leaving stage n. Again, a total condenser has been assumed in the above equations. The unknown $x_m(n)$ can be eliminated from equation (20) by using the following equation

$$x_m(n) = 1 - \sum_{j=1}^{m-1} x_j(n). \tag{21}$$

Equation (20) now becomes

$$g_m(n) = [L(n) + D]\alpha(n + 1) - L(n)\beta(n) - D\beta(0) - Q_c = 0, \quad n = 1, 2, \ldots, (f - 1) \tag{19b}$$

with

$$\partial(n) = k_m(n)H_m(n) + \sum_{j=1}^{m-1} (x_j(n)[k_j(n)H_j(n) - k_m(n)H_m(n)]) \tag{22}$$

$$\beta(n) = h_m(n) + \sum_{j=1}^{m-1} (x_j(n)[h_j(n) - h_m(n)]). \tag{23}$$

For the stripping section, the material and enthalpy balances were obtained by considering the reboiler and any stage $(n + 1)$. After elimination, the resulting two equations for the stripping section are

$$g_i(n) = [L(n) - B]k_i(n + 1)x_i(n + 1) + Bx(N + 1) - L(n)x_i(n) = 0,$$

$$i = 1, 2, \ldots, m - 1; \quad n = N, N - 1, \ldots, f \tag{24a}$$

$$g_m(n) = [L(n) - B]\alpha(n + 1) - L(n)\beta(n) - D\beta(0) - Q_c + F\sum_{j=1}^{m} x_{jf}h_{jf} = 0,$$

$$n = N, N - 1, \ldots, f. \tag{24b}$$

Equations (19) and (24) are the desired equations. They constitute m nonlinear first order difference equations. The m unknowns are $L(n)$ and $x_i(n)$, $i = 1, 2, \ldots, (m - 1)$. Notice that equations (19) and (24) are a mixed simultaneous system of algebraic and difference equations. The equations are algebraic in $L(n)$ since only an algebraic quantity $L(n)$ appears in these equations. They are first order difference equations in $x_i(n)$ since both $x_i(n)$ and $x_i(n + 1)$ appear in these equations. Since $L(n)$ is an algebraic quantity and also since $L(0)$ is given, no equation is needed for the zeroth stage for $L(n)$. For $x(n)$, the zeroth stage equation can be represented by

$$g_i(0) = x_i(0) - k_i(1)x_i(1), \quad i = 1, 2, \ldots, (m - 1). \tag{25}$$

Equations (19), (24), and (25) represent the complete column including the condenser and the reboiler. The condenser duty, Q_c, is represented by equation (3). The unknown $x_m(0)$ can again be eliminated from equation (3) by using equation (21). The resulting equation is

$$Q_c = V(1)[H_m(1) - h_m(0)] + V(1)\sum_{j=1}^{m-1} x_j(0)[H_j(1) - h_j(0) - H_m(1) + h_m(0)]. \tag{26}$$

Instead of solving the above system in a stage by stage fashion from the condenser to the reboiler, the problem will be solved in two sections with the boundary conditions at the feed stage. In other words, the calculations will commence at each end of the column and continue in a stage by stage fashion until the feed plate. In order to use the same initial conditions at both end of the column, the following equation can be added to the above system of difference equations

$$Fx_{if} = Dx_i(0) + Bx_i(N + 1), \quad i = 1, 2, \ldots, (m - 1). \tag{27}$$

Equations (19), (24), (25) and (27) constitute the system of difference equations over the entire length or stages of the problem. Notice that equation (27) is a first-order difference equation for our purpose. The boundary conditions for this system of equations can be obtained by matching the results at the feed plate.

$$\bar{k}_i(f)\bar{x}_i(f) = k_i(f)x_i(f), \quad i = 1, 2, \ldots, (m - 1), \tag{28}$$

where $\bar{x}$ represents the stripping section results and x represents the rectifying, section results. The above system of equations can again be solved by quasilinearization. Equations (19) and (24) can be represented symbolically by

$$g(x(0), x(n), z(n + 1), x(N + 1)) = 0, \quad n = 1, 2, \ldots, N, \tag{29}$$

where g and $z(n + 1)$ represent m dimensional vectors with components $g_1, g_2, \ldots, g_m$ and

$x_1(n + 1), x_2(n + 1), \ldots, x_{m-1}(n + 1), L(n)$, respectively. The x's represent $(m - 1)$ dimensional vectors. Equation (29) can be linearized as

$$g_k + J_{x(0)}[x_{k+1}(0) - x_k(0)] + J_{x(n)}[x_{k+1}(n) - x_k(n)]$$
$$+ J_{z(n+1)}[z_{k+1}(n + 1) - z_k(n + 1)] + J_{x(N+1)}[x_{k+1}(N + 1) - x_k(N + 1)] = 0, \qquad (30)$$

where $J_{z(n+1)}$ represents an $m \times m$ matrix and the other Jacobians are $mx(m - 1)$ matrices. The elements of the Jacobians can be obtained in the same way as before. Again, the functions $k_i(n)$ and $H_i(1)$ are not considered in the linearization. Since $k_i(n)$ is not considered in linearization, both equations (25) and (27) are linear equations. The general solutions for the linear equations (25), (27) and (30) can be represented by

$$x_{i,k+1}(n) = x_{ip,k+1}(n) + \sum_{j=1}^{m-1} a_j x_{ihj,k+1}(n) \qquad (31)$$

$$i = 1, 2, \ldots, (m - 1); \quad n = 0, 1, 2, \ldots, N + 1.$$

Since $L(n)$ appears only as an algebraic quantity, the solutions for $L(n)$ is

$$L_{k+1}(n) = L_{p,k+1}(n), \quad n = 1, 2, \ldots, n. \qquad (32)$$

However, equation (32) is correct only if correct values of $x_i(0)$, $i = 1, 2, \ldots, (m - 1)$ are used as the initial condition for the particular solution. Since $x_i(0)$'s are unknown quantities whose values are the desired results, some approximate values must be used for $x_i(0)$. Thus, equation (32) is not exact until convergence is obtained. To avoid this difficulty, any reasonable set of values were used for $x_p(0)$ and the following equation is used to obtain the solution of $L(n)$ during the first few iterations

$$L_{k+1}(n) = L_{p,k+1}(n) + \sum_{j=1}^{m-1} a_j L_{hj,k+1}(n), \qquad (33)$$

with $n = 1, 2, \ldots, N$. The $(m - 1)$ integration constants can be obtained by substituting equation (31) into the boundary conditions. Equation (28). Once the $(m - 1)$ a's are obtained, the general solution can be obtained by using equations (31)–(33).

Using the numerical values listed in equation (11) and using the following initial approximations

$$x_{1,k=0}(n) = 0.05, \quad x_{2,k=0}(n) = 0.15, \quad x_{3,k=0}(n) = 0.25, \quad x_{4,k=0}(n) = 0.20, \qquad (34)$$

for all n, and

$$L_{k=0}(n) = 126.2, \quad n = 1, 2, \ldots, f - 1$$
$$L_{k=0}(n) = 226.2, \quad n = f, f + 1, \ldots, N, \qquad (35)$$

the results listed in Table 4 is obtained. Notice that the initial approximations used are very approximate and 126.2 is the value of $L(0)$.

Table 4. Convergence rates of distillate composition and $L(1)$

Iteration	$x_1(0)$	$x_2(0)$	$x_3(0)$	$x_4(0)$	$L(1)$
0	0.05	0.15	0.25	0.20	126.2
1	0.1584	0.3857	0.4732	0.0003	127.4
2	0.1440	0.3601	0.4735	0.0494	103.2
3	0.0963	0.2934	0.4724	0.0681	120.3
4	0.1056	0.3021	0.4663	0.0611	125.3
5	0.1025	0.2999	0.4704	0.0673	124.8
6	0.1022	0.2998	0.4712	0.0691	123.8
7	0.1022	0.2999	0.4717	0.0707	122.9
8	0.1022	0.2999	0.4721	0.0717	122.3
9	0.1022	0.3000	0.4722	0.0722	122.0
10	0.1022	0.3000	0.4723	0.0724	121.9

For the homogeneous solutions, the same values listed in Table 1 are used as the initial conditions for all iterations for $x_{ihj,k+1}(0)$, $i,j = 1, 2, 3, 4$. However, since we wish to obtain the solution for $L(n)$ simultaneously, the initial conditions used for the particular solutions are

$$x_{ip,k+1}(0) = x_{i,k+1}(0), \quad i = 1, 2, \ldots, (m-1). \tag{36}$$

In other words, the general solution of the previous iteration is used as the particular solution initial condition of the current iteration for all the iterations. Notice that inspite of the very rough initial approximations, the convergence rates obtained are much faster than those obtained earlier. Furthermore, since only $(m-1)$, not m, homogeneous solutions are needed, the computation time required is also reduced.

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