CHAPTER V

NUMERICAL SOLUTION OF THE TOPPING COLUMN MODELS

The mathematical models derived in Chapter IV are all described by a system of nonlinear equations in the form

$$\mathbf{f}(\mathbf{x}) = 0 \tag{63}$$

where $\mathbf{f}$ and $\mathbf{x}$ are column vectors, defined as

$$\mathbf{f} = [\ f_0,\ f_1, \ldots,\ f_N,\ g_1,\ g_2, \ldots,\ g_N\ ]^T \tag{64}$$

$$\mathbf{x} = [\ \theta_0,\ \theta_1, \ldots,\ \theta_N,\ T_1,\ T_2, \ldots,\ T_N\ ]^T \tag{65}$$

One practical method for solving Eq.(63) is the Newton-Raphson method, which consists of the iteration of the following Newton-Raphson equation

$$\mathbf{J}_k \Delta \mathbf{x}_k = -\ \mathbf{f}(\mathbf{x}_k) = -\ \mathbf{f}_k \tag{66}$$

where $\mathbf{J}_k$ is the Jacobian matrix

$$\mathbf{J}_k = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \vdots \\ \frac{\partial f_n}{\partial x_1} \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} .$$

The partial derivatives appearing in J_k are evaluated using the current set of values of the variables $\mathbf{x}_k$. After Eq.(66) has been solved for $\Delta \mathbf{x}_k$, the new values $\mathbf{x}_{k+1}$ for the next iteration are given by

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \Delta \mathbf{x}_k \quad (67)$$

Convergence of the method can often be promoted by requiring that the new $\mathbf{x}_{k+1}$ satisfies the inequality

$$[\ \Sigma\ f_i^2(\mathbf{x}_{k+1})\ ]^{\frac{1}{2}} \ < \ [\ \Sigma\ f_i^2(\mathbf{x}_k)\ ]^{\frac{1}{2}} \quad (68)$$

After an appropriate $\mathbf{x}_{k+1}$ has been determined, the iterative procedure is repeated until convergence is achieved. The method thus requires that the Jacobian matrix defined by Eq.(66) be evaluated at each step of iteration. In the solution of large sets of equations, coding of the Jacobian matrix can prove to be a formidable task if analytical expressions of the partial derivatives be desired. The problem can be eliminated by evaluating the partial derivatives numerically at the expense of significantly more computer time. Hence quasi-Newton methods have been proposed to circumvent these problems.

5.1 Modified Newton-Raphson Method with Broyden-Householder Formula

Tomich (22) was the first to apply Broyden's method to the solution of distillation problem. Broyden's method numerically approximates the partial derivatives appearing in the Jacobian matrix with the formula

$$\frac{\partial f_i}{\partial x_j} = \frac{f_i(x + \Delta x_j) - f_i(x)}{\Delta x_j} \qquad (69)$$

where the approximation error is of the order $0(\Delta x)$.

If x_{k+1} does not satisfy the inequality equation (68), a scalar $0 < s_k \leq 1$ that minimizes the euclidean norm of $f(x_{k+1})$ is used. In this case

$$x_{k+1} = x_k + s_k \Delta x_k \qquad (70)$$

Broyden (65) suggested that s_k be determined from

$$s_k = \frac{(1 + 6n)^{\frac{1}{2}} - 1}{3n} \qquad (71)$$

where

$$n = \frac{\Sigma f_i^2(x_k + \Delta x_k)}{\Sigma f_i^2(x_k)} \qquad (72)$$

Broyden further proposed that instead of employing the exact Jacobian matrix at each step of iteration an approximation be used. He presented a formula to sequentially update the approximate Jacobian at each step as follows:

$$J_{k+1} = J_k + \frac{[f_{k+1} - (1 - s_k)f_k]\Delta x_k^T}{s_k \Delta x_k^T \Delta x_k} \qquad (73)$$

Davidon (66) later proposed the variable metric or quasi-Newton methods defined by

$$x_{k+1} = x_k + s_k H_k f_k \qquad (74)$$

where H_k is defined as the minus inverse matrix of J_k.

An original estimate H_0 is provided, then the Broyden-Householder's algorithm (65) is used to update H_k sequentially as follows

$$H_{k+1} = H_k - \frac{(H_k y_k + s_k \Delta x_k) \Delta x_k^T H_k}{\Delta x_k^T H_k y_k} \tag{75}$$

where $y_k = f_{k-1} - f_k$. Lucia (67) presented a discussion that indicated that the Broyden-Householder's algorithm when modified to include periodical Jacobian restart, is superlinearly convergent.

5.2 Algorithm of Developed Computer Program

In this work, the algorithm of the developed simulation program is based on Broyden-Householder's with periodical restart. The algorithm is as follows:

Step 1: Set k=0 and choose a starting point x_0 by assuming a set of the temperatures, T_j and the flow ratios, $(V_j/L_j)_a$. Assume all of the θ_j to be equal to 1.

Step 2: Compute $f(x_k)$ as described in 4.2.6.

Step 3: Set iter=1. As a first approximation of the elements of J_k use the formula

$$\frac{\partial f_i}{\partial x_j} = \frac{f_i(x_j + h_j) - f_i(x_j)}{h_j} \tag{76}$$

where h_j is roughly equal to $0.001x_j$. Then compute

$$H_k = - J_k^{-1}$$

Step 4: Using the latest iterative values of H_k and f_k, compute

$$\Delta x_k = H_k f_k \tag{77}$$

Step 5: Find a s_k such that the Euclidean norm of $f(x_k + s_k \Delta x_k)$ is a minimum among s_k = 0.05, 0.10, 0.15,..., 1.00. If the norm cannot reduced at all assumed values of s_k, return to step 3 and reevaluate the elements of J_k on the basis of x_k. Otherwise, go to the next step.

Step 6: Set

$$x_{k+1} = x_k + s_k \Delta x_k$$

$$f_{k+1} = f(x_{k+1})$$

Step 7: Test f_{k+1} for convergence, if $||f(x_{k+1})||_2 < e$, stop. Otherwise, set iter=iter+1. If iter=5, return to step 3.

Step 8: Compute

$$y_k = f_{k+1} - f_k$$

and

$$H_{k+1} = H_k - \frac{(H_k y_k + s_k \Delta x_k) \Delta x_k^T H_k}{\Delta x_k^T H_k y_k}$$

Step 9: Set k=k+1 and set the temperatures and the flow ratios equal to the most recent values found in Step 6. Reset all the θ_j = 1 and go to step 4.

5.3 Testing the Computer Program on a Known Problem

The computer program developed on the above algorithm was tested on a problem originally solved by Cecchetti et al (39) and

Hess et al.(40). The objective was to debug as well as to check the performance of the program. The problem was based on data from field tests of an topping column as shown in Fig.25. The theoretical analogue column shown in Fig.26 is taken to be the same as that proposed by Cecchetti et al.

The physical properties (normal boiling points, densities and molecular weights) of the 34 pseudocomponents selected to represent the true boiling point curves of the feed, distillate and sidestreams are given by Cecchetti et al. Curve fits of the K-values and enthalpies of pseudocomponents are presented elsewhere (14). On the basis of these data, a feed having the molar compositions and total flow rate shown in Table 6 was used by Cecchetti et al. For the theoretical analogue column shown in Fig.26, its specifications are given in Table 6 and the plate location variables as defined in 4.2 are as follows:

Plate	NW(i)	= 6,11,16,23
	NV(i)	= 5,10,15,22
	NP(i)	= 19
	NQ(i)	= 18
	NF	= 27
	NT	= 28
	NTOP(i)	= 29,32,34,36
	NBOT(i)	= 31,33,35,37

The complete sets of total and component material balances are obtained in the manner described in 4.2.2-4.2.3 and represented

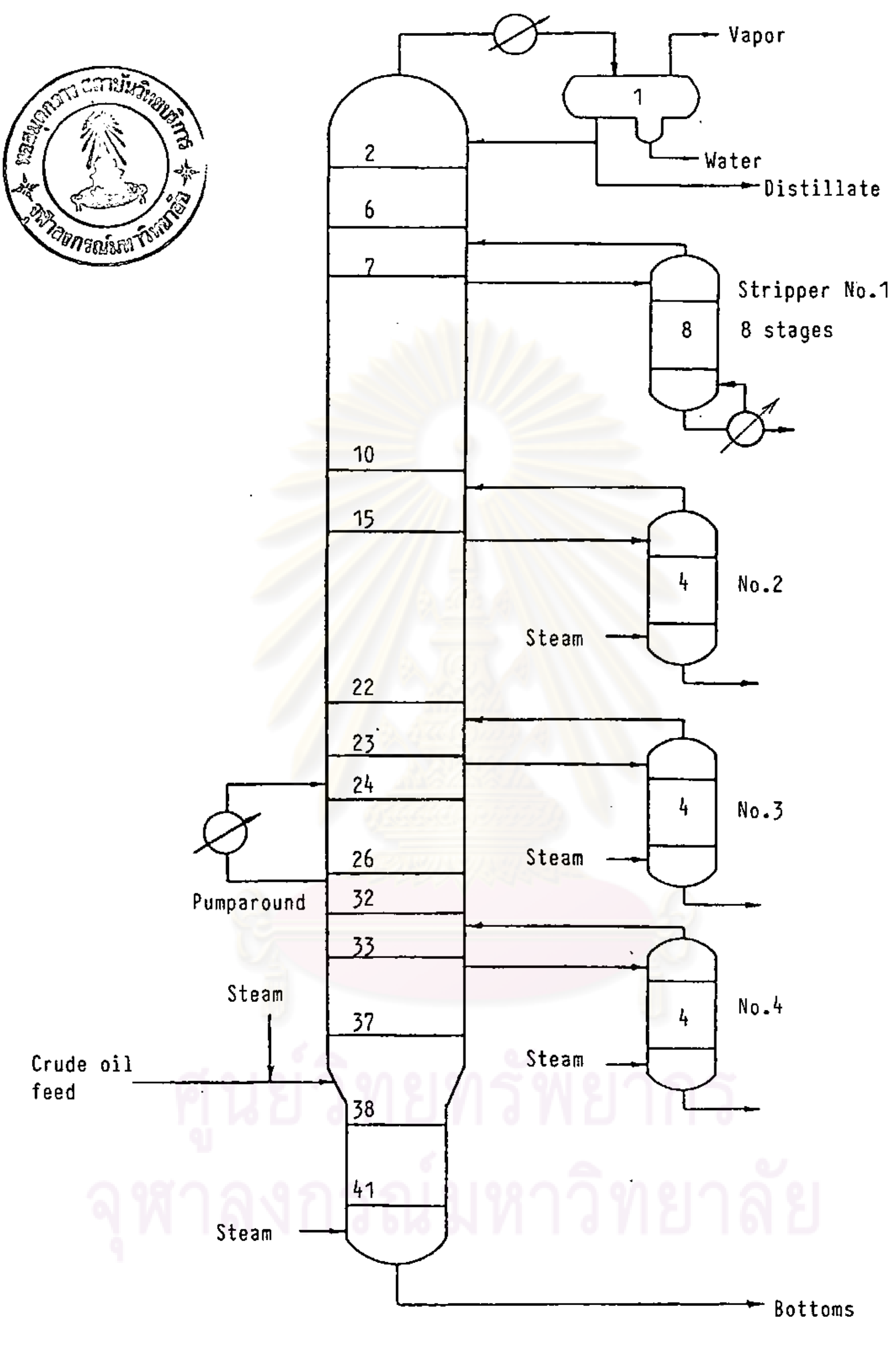

Fig.25 Actual tray numbers in topping column and sidestrippers.

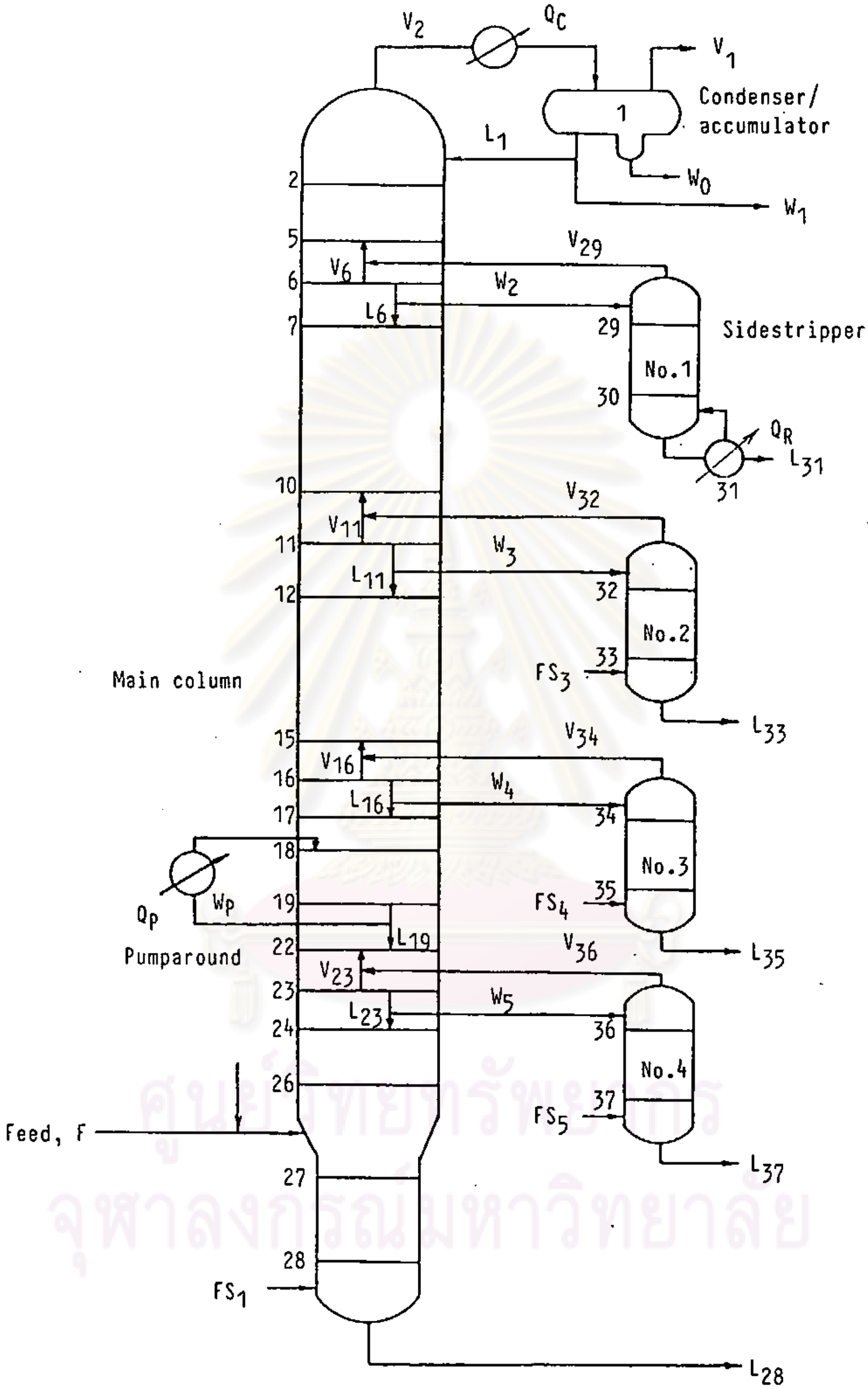

Fig.26 Theoretical trays corresponding to system in Fig.25, obtained by Cecchetti et al. (39).

Table 6 Composition of the feed stream and other specifications for the theoretical analogue column shown in Fig.26 (40).

Component	Feed(lb.mol/h)	Other specifications
1	0.73000×10^{1}	The hydrocarbon feed enters the column at 637°F with 69.038% of feed vaporized and a total enthalpy of 219.890×10^{6} Btu/h. The steam enters the main column and the sidestrippers as superheated steam at 532°F at the rates FS_1 = 66, FS_3 = 6.94, FS_4 = 26.8, and FS_5 = 15.8 lb.mol/h. The sidestrippers are withdrawn at the rates L_{31} = 293.66, L_{33} = 122.58, L_{35} = 329.57, and L_{37} = 107.70 lb.mol/h. The pumparound stream is withdrawn at the rate of W_p = 8223 lb.mol/h and the intercooler duty Q_p = 18.0×10^{6} Btu/h. The reflux ratio L_1/V_1 = 10.95 and the boilup ratio V_{31}/L_{31} = 0.13245. The pressure in the accumulator is 23.1 psia, and the pressure on plate 28 is 29.24 psia. An equal pressure drop per plate may be assumed for the main column and the sidestrippers. The pressure on the top plate of each sidestripper may be taken equal to the pressure of the plate in the main column from which the sidestream feed to the stripper originated.
2	0.25700×10^{2}	
3	0.38000×10^{2}	
4	0.43800×10^{2}	
5	0.95700×10^{2}	
6	0.71400×10^{2}	
7	0.63300×10^{2}	
8	0.63300×10^{2}	
9	0.76250×10^{2}	
10	0.72250×10^{2}	
11	0.43950×10^{2}	
12	0.43950×10^{2}	
13	0.86500×10^{2}	
14	0.29400×10^{2}	
15	0.29400×10^{2}	
16	0.51000×10^{2}	
17	0.34000×10^{2}	
18	0.34000×10^{2}	
19	0.30640×10^{2}	
20	0.30650×10^{2}	
21	0.67600×10^{2}	
22	0.65600×10^{2}	
23	0.42400×10^{2}	
24	0.71200×10^{2}	
25	0.67500×10^{2}	
26	0.12780×10^{3}	
27	0.11360×10^{3}	
28	0.97100×10^{2}	
29	0.81200×10^{2}	
30	0.67800×10^{2}	
31	0.47700×10^{2}	
32	0.57300×10^{2}	
33	0.29600×10^{2}	
34	0.28300×10^{2}	
35	0.26400×10^{2}	

Total feed = 0.22032×10^{4} lb.mol/h

$$
C = \begin{array}{l}
b_1 \quad c_1 \quad 0 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 0 \\
a_2 \quad b_2 \quad c_2 \quad 0 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 0 \\
0 \quad a_3 \quad b_3 \quad c_3 \quad 0 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 0 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 \cdots 0 \quad a_5 \quad b_5 \quad c_5 \quad 0 \cdots 0 \quad c_{5,29} \quad 0 \cdots\cdots\cdots\cdots\cdots 0 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 \cdots\cdots 0 \quad a_{10} \quad b_{10} \quad c_{10} \quad 0 \cdots 0 \quad c_{10,32} \quad 0 \cdots\cdots\cdots\cdots 0 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 \cdots\cdots\cdots 0 \quad a_{15} \quad b_{15} \quad c_{15} \quad 0 \cdots 0 \quad c_{15,34} \quad 0 \cdots\cdots\cdots 0 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 \cdots\cdots\cdots\cdots 0 \quad a_{22} \quad b_{22} \quad c_{22} \quad 0 \cdots 0 \quad c_{22,36} \quad 0 \cdots\cdots 0 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
0 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 0 \quad a_{36} \quad b_{36} \quad c_{36} \\
0 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 0 \quad 0 \quad a_{37} \quad b_{37}
\end{array}
$$

Fig.27 Abbreviated display of the component material balance matrix C_i.

Table 7 Elements of matrices for total material balances.

I. Elements of the square matrix **T**

$a_j = 1$, $j = 2,3,\ldots,28$

$b_1 = -(1+R_1+R_0R_1)$

$b_j = -(1+R_j)$, $j = 2,3,\ldots,28$

$c_j = R_{j+1}$, $j = 1,2,\ldots,27$

II. Elements of the column vector **F**

$f_j = 0$ except as follows

$f_1 = -W_1$, $f_5 = R_{29}L_{29}$, $f_6 = -W_2$, $f_{18} = -W_P$

$f_{26} = V_F$, $f_{10} = R_{32}L_{32}$, $f_{11} = -W_3$, $f_{19} = W_P$

$f_{27} = L_F$, $f_{15} = R_{34}L_{34}$, $f_{16} = -W_4$

$f_{28} = FS_1$, $f_{22} = R_{36}L_{36}$, $f_{23} = -W_5$

where

$L_{29} = (1+R_{30})L_{30} - R_{31}L_{31}$, $W_2 = (1+R_{29})L_{29} - R_{30}L_{30}$

$L_{30} = (1+R_{31})L_{31}$, $W_3 = (1+R_{32})L_{32} - R_{33}L_{33}$

$L_{32} = (1+R_{33})L_{33} - FS_3$, $W_4 = (1+R_{34})L_{34} - R_{35}L_{35}$

$L_{34} = (1+R_{35})L_{35} - FS_4$, $W_5 = (1+R_{36})L_{36} - R_{37}L_{37}$

$L_{36} = (1+R_{37})L_{37} - FS_5$

which are obtained by sequential substitutions.

Table 8 Elements of matrices for component material balances.

I. Elements of the square matrix $\mathbf{C}_i$

i) For water on stages j = 1 and j = 2

$$b_1 = -(1+A_{0c}) \quad ,c_1 = 1$$

$$a_2 = 0, \quad b_2 = -(1+A_{2c}) \quad ,c_2 = 1$$

ii) For all hydrocarbon components on stages j = 2 through j = 37 and for water on stages = 3 through j = 37.

$a_j = A_{j-1,i}$ for all j except for j = 29,32,34,36, and for these values of j, $a_j = 0$.

$$a_{29,6} = (W_2/L_6)A_{6i} \quad , \quad a_{32,11} = (W_3/L_{11})A_{11i}$$

$$a_{34,16} = (W_4/L_{16})A_{16i} \quad , \quad a_{36,23} = (W_5/L_{23})A_{23i}$$

$b_j = -(1+A_{ji})$ for all j except for j = 1,6,11,16,19,23 and for these values of j:

$b_j = -[1+A_{ji}(1+W/L_j)]$, where $W = W_1$ (for j = 1), $W = W_2$ (for j = 5), $W = W_3$ (for j = 10), $W = W_4$ (for j = 16), $W = W_p$ (for j = 19), and $W = W_5$ (for j = 23).

$c_j = 1$ for all j except for j = 18, and for j = 18, $c_{18} = 1+(W_p/L_{19})A_{19i}$.

$$c_{5,29} = c_{10,32} = c_{15,34} = c_{22,36} = 1$$

II. Elements of the column vector $\mathbf{f}_i$

$f_{ji} = 0$ except for the following:

$$f_{26i} = v_{Fi} \; , \; f_{27i} = l_{Fi} \; ,$$

$$f_{28c} = FS_1 \; , \; f_{33c} = FS_3 \; , \; f_{35c} = FS_4 \; , \; f_{37c} = FS_5 .$$

Table 9 Nonzero values of the coefficients of the generalized enthalpy-balance function (Eq.60-62).

Stage	C_{1j}	C_{2j}	C_{3j}	C_{4j}	C_{5j}	C_{6j}	C_{7j}
1	1						1
2	1	1					
3	1	1					
4	1	1					
5	1	1	1				
6	1	1					
7	1	1					
8	1	1					
9	1	1					
10	1	1	1				
11	1	1					
12	1	1					
13	1	1					
14	1	1					
15	1	1	1				
16	1	1					
17	1	1					
18	1	1		W_p/L_{19}			1
19	1	1					
20	1	1					
21	1	1					
22	1	1	1				
23	1	1					
24	1	1					
25	1	1					
26	1	1			1		
27	1	1				1	
28		1			1		
29	1			W_2/L_6			
30	1	1					
31		1					-1
32	1			W_3/L_{11}			
33		1			1		
34	1			W_4/L_{16}			
35		1			1		
36	1			W_5/L_{23}			
37		1			1		

Table 10 Initial and final column profiles obtained by the present computer program and published by Hess et al.(40).

Plate No.	Temperature, °F			Liquid flow rate, lb mol/h			Vapor flow rate, lb mol/h		
	Initial	Final	Hess	Initial	Final	Hess	Initial	Final	Hess
1	100.00	111.85	111.64	2178.0	2126.7	2129.8	198.90	195.48	194.50
2	122.22	167.08	116.79	2178.0	2107.0	2108.9	2862.0	2814.1	2816.1
3	144.44	192.83	192.56	2178.0	2052.0	2053.4	2862.0	2794.3	2795.2
4	166.67	210.98	210.74	2178.0	1984.0	1985.4	2862.0	2739.3	2739.7
5	188.89	228.06	227.83	2178.0	1893.3	1894.9	2862.0	2671.3	2671.6
6	211.11	247.67	247.41	1864.6	1461.1	1463.3	2825.3	2561.4	2561.5
7	233.33	272.82	272.47	1864.6	1357.6	1359.9	2825.3	2442.2	2443.3
8	255.56	297.35	296.95	1864.6	1301.4	1303.0	2825.3	2339.0	2340.0
9	277.78	316.61	316.27	1864.6	1280.2	1281.4	2825.3	2282.5	2283.1
10	300.00	329.73	329.46	1864.6	1264.1	1265.5	2825.3	2261.3	2261.4
11	322.22	339.30	339.07	1728.5	1100.9	1102.5	2818.4	2224.8	2225.0
12	355.55	348.25	348.00	1728.5	1059.3	1061.2	2818.4	2197.6	2198.2
13	366.67	357.96	357.68	1728.5	1001.5	1003.4	2818.4	2156.1	2156.8
14	388.89	370.14	369.84	1728.5	920.23	922.26	2818.4	2098.3	2099.1
15	411.11	386.94	386.60	1728.5	808.78	812.16	2818.4	2017.0	2017.9
16	433.33	411.03	410.45	1360.1	323.29	329.69	2791.6	1840.0	1842.2
17	455.55	441.16	439.86	1360.1	277.80	285.59	2791.6	1722.6	1728.1
18	477.78	455.55	453.90	2183.1	158.91	1607.8	2791.6	1677.1	1684.0
19	500.00	488.46	486.45	1360.1	858.57	879.87	2791.6	2165.4	2183.3
20	522.22	510.64	508.06	1360.1	836.42	859.71	2791.6	2257.9	2278.3
21	544.44	523.76	520.82	1360.1	786.80	816.99	2791.6	2235.7	2258.1
22	566.67	535.00	531.37	1360.1	711.65	759.57	2791.6	2186.1	2251.4
23	588.89	547.70	542.52	1234.7	486.69	554.13	2775.8	2078.0	2124.4

Table 10 (continued)

Plate No.	Temperature, °F			Liquid flow rate, lb mol/h			Vapor flow rate, lb mol/h		
	Initial	Final	Hess	Initial	Final	Hess	Initial	Final	Hess
24	611.11	563.28	556.74	1234.7	466.58	462.72	2775.8	1978.4	2044.5
25	633.33	576.88	572.98	1234.7	345.16	354.27	2775.8	1898.3	1953.1
26	655.55	588.75	593.34	1234.7	162.70	154.74	2775.8	1836.9	1844.6
27	677.78	621.56	629.46	1916.8	814.67	811.63	1254.7	133.38	123.98
28	700.00	617.99	626.51	728.12	777.47	778.86	1254.7	103.21	98.768
29	211.11	256.72	256.46	313.4	326.69	326.68	36.63	19.688	19.775
30	233.33	261.30	261.04	313.4	332.56	332.53	36.53	32.942	33.020
31	255.56	267.08	266.80	276.8	293.75	293.66	36.63	38.814	38.866
32	322.22	332.14	331.89	136.1	130.74	130.74	6.94	20.434	20.442
33	344.44	322.20	321.95	136.1	122.58	122.58	6.94	15.102	15.105
34	433.33	404.97	404.36	368.4	352.43	352.74	26.80	65.521	65.626
35	455.55	396.19	395.54	368.4	329.32	329.59	26.80	49.911	49.969
36	588.89	541.22	535.40	125.4	118.22	117.97	15.80	32.940	33.464
37	611.11	530.92	524.46	125.4	108.21	107.70	15.80	25.809	26.072

by matrix equations. An abbreviated display of the elements of the above matrices is shown in Fig.27. A complete definition of the elements is given in Tables 7 and 8.

The sets of independent functions F_j and G_j are formulated using Eq.(54-56,60-62), and the coefficients C_{1j} to C_{7j} have these nonzero values given in Table 9.

The sets of temperatures and flow rates obtained by the present computer program are presented in Table 10. The table also shows that the obtained results agreed well with those published by Hess et al.(40).