LETTERS TO THE EDITOR

To the Editor:

I would make some remarks about the article "A Modified Naphtali-Sandholm Method for General Systems of Interlinked, Multistaged Separators" (AIChE J., *24*, 1131, 1978) The subject is extremely interesting for the well known efficiency of Newton-Raphson method to solve algebraic equations. I think, however, that the solving procedure proposed by the Authors for the linear equations system (resulting by application of Newton method to interlinked columns with non-standard specifications) is not completely adequate. In detail I think that:

1) It is not possible to utilize the method when specifications are not standard. Let us reflect on the example in the article: the condenser duty is considered as variable, and the temperature T_4 is fixed. In the text is not clear if the energy balance equation is removed from the system (and solved apart for the variable δQ_1) or not.

The first solution is not general: it is possible only if heat Q_j (which appears only in the energy equation) is introduced as variable. The second solution, which implies a change of matrices A,B,C dimensions, creates heavy problems in programming. Both solutions don't allow to solve the system according to the proposed method, because the new row introduced for the T_4 = const specification has zero coefficients in submatrix B_1 (corresponding to variables δx_{1j}, δy_{1j}, δV_1, δL_1, δT_1, and, eventually, δQ_1).

So it is impossible to perform step 1: $p_1 \leftarrow B_1^{-1}C_1$; $q_1 \leftarrow B_1^{-1}F_1$.

2) Auxiliary memories utilization is not optimized.

The elimination of under-tridiagonal submatrices requires repeated readings of memory where submatrices p (step 6 and step 9) are written. (NOTE: in step 6 there is a printing error: instead of "reset $\beta = -p_{M-1}$" it must be read "reset $\beta = -p_{M-1,M}$").

The difficulty of the problem increases when on the same row there are several submatrices lying under the tridiagonal (several bypassing converging to the same tray). Moreover the method becomes very heavy when submatrices out the tridiagonal are arranged as E and S in figure 1.

Matrix S, during this method's steps, causes the introduction of submatrices shown in figure 1 as $S°$. Thus we have a new matrix where row of submatrix E and column of submatrix S cross each other and this new submatrix must be removed, too.

In order to limit I/O time of auxiliary memories, I think we must read/write as less as possible the memory in which rows without terms under the tridiagonal are stored. This may be done by reversing the method's procedure: instead of removing submatrices E with a backward method, matrices E are eliminated by a forward method not requesting iterative reading of preceding rows.

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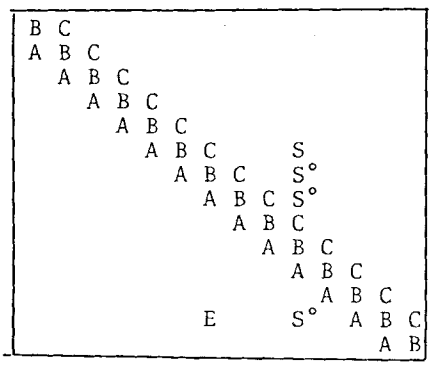

Figure 1.

Reply

1. Standard specifications are the condenser duty, Q_1, and the reboiler duty, Q_N. In the example in our paper, the specification equation $T_4 = T_{spec}$ replaces the energy-equation, E_1 (not E_4), and the specification equation $V_{10} = V_{spec}$ replaces the energy equation, E_N. Such replacements are easily made in a computer program, and do not change the size of the Jacobian matrix or the sizes of any of the A, B, and C submatrices. In the Naphtali-Sandholm paper, they also consider the case of specifying the temperature of a specific tray, e.g. T_4. But to preserve the block tridiagonal structure of the Jacobian matrix, they use the specification equation $T_j = T_{spec}$ as a replacement for the corresponding energy equation, E_j (not E_1). Thus, they obtain the desired value of T_j by considering plate J as non-adiabatic and determining the necessary rate of heat transfer to or from that plate. Our procedure, which is more general, must be used with care because it is certainly possible to specify a T_j that is impossible. Of course, the same difficulty is true for the Naphtali-Sandholm method, but by only permitting a Q_j other than zero they give more latitude in the T_j specification.

2. Ferraris claims that there is a misprint in Table 1 of our paper. He is correct; in fact there are two misprints, including the one he cites. Lines 4 and 5 of Step 6 should read:

$$\begin{aligned} &\text{reset } \beta = -p_{M-1,M}; \\ &\text{iterate on } \beta \leftarrow -p_i\beta \\ &\text{from } i = M-2 \text{ to } i = J; \\ &p_{P,M} \leftarrow B_P A_{P,J}\beta \end{aligned}$$

Ferraris also claims that our method becomes more difficult and very heavy for certain matrix structures other than the one shown in Figure 3 of our paper. The algorithm given in Table 1 of our paper

TABLE 1. EQUATIONS FOR FORWARD SUBSTITUTION TO OBTAIN FIGURE 2 FROM FIGURE 1

p	q
$p_1 = B_1^{-1}C_1$	$q_1 = B_1^{-1}F_1$
$p_{1,4} = B_1^{-1}C_{1,4}$	
$p_2 = (B_2 - A_2p_1)^{-1}C_2$	$q_2 = (B_2 - A_2p_1)^{-1}(F_2 - A_2q_1)$
$p_{2,4} = -(B_2 - A_2p_1)^{-1}A_2p_{1,4}$	
$p_3 = (B_3 - A_3p_2)^{-1}(C_3 - A_3p_{2,4})$	$q_3 = (B_3 - A_3p_2)^{-1}(F_3 - A_3q_2)$
$p_i = (B_i - A_ip_{i-1})^{-1}(C_i)$ $i = 4,5,6$	$q_i = (B_i - A_ip_{i-1})^{-1}(F_i - A_iq_{i-1})$
$p_7 = (B_7 - A_7p_6 + A_{7,2}\beta_7)^{-1}C_7$	$q_7 = (B_7 - A_7p_6 + A_{7,2}\beta_7)^{-1}(F_7 - A_7q_6 + A_{7,2}\bar{\beta}_7)$

where: $\beta_7 = p_{2,4}p_4p_5p_6 - p_2p_3p_4p_5p_6$

and $\bar{\beta}_7 = -q_2 + p_2q_3 - p_2p_3q_4 + p_2p_3p_4q_5 - p_2p_3p_4p_5q_6 + p_{2,4}q_4 - p_{2,4}p_4p_5 + p_{2,4}p_4p_5q_6$

$$q_8 = (B_8 - A_8p_7)^{-1}(F_8 - A_8q_7)$$

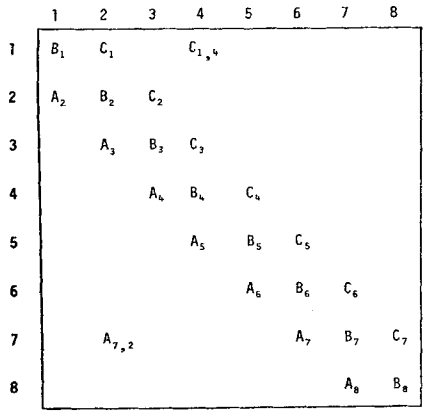

Figure 1. Example of starting matrix for case 3.

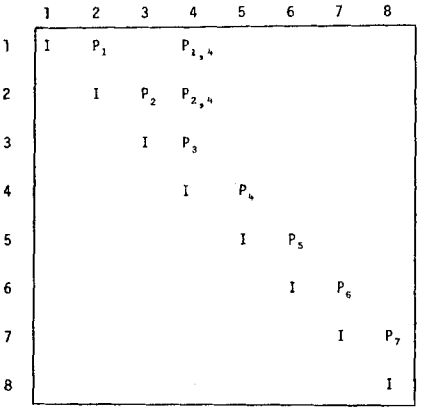

Figure 2. Matrix of Figure 1 after forward substitution.

applies only to the matrix structure given in Figure 3 of our paper, and thus is illustrative only. Similar algorithms are readily developed for other matrix structures, including the cases mentioned by Ferraris, such as: (1) where two or more nonzero blocks occur in the same column and above the tridiagonal blocks; (2) where two or more nonzero blocks occur in the same row and below the tridiagonal blocks; and (3) where a row containing a nonzero below-the-tridiagonal block and a column containing a nonzero, above-the-tridiagonal block intersect at a block that lies below the tridiagonal blocks. For example, consider Case 3 with the matrix structure shown in the attached Figure 1. The application of our technique leads to an algorithm, from which the equations for the resulting p and q elements shown in the attached Figure 2 are as listed in the attached Table 1. It does not seem to me that these equations are difficult or heavy. In fact, these equations, as well as those of Table 1 of our paper, are precisely those obtained by an LU decomposition. The new submatrix $S°$ mentioned by Ferraris does not even enter the equations.

When many nonzero, off-tridiagonal blocks occur in the matrix structure then as discussed in the paper, "An Optimal Arrangement of Simultaneous Linearized Equations for General Systems of Interlinked, Multistaged Separators" by Hildalgo, Correa, Gomez, and me, which appears in this issue of the *AIChE Journal*, it may be more efficient to utilize standard Gaussian elimination or LU decomposition techniques rather than our technique. However, no study has been reported that quantitatively shows at what degree of matrix density it is best to just use standard techniques.

Ferraris is also concerned about I/O time of auxiliary memories. While this may be of concern with computers of very small memory, it is of little concern with today's modern computers that have either a virtual memory or a large main memory. With such computers, which are very common, the removal of submatrix E with a backward method is efficient, accurate, and presents no difficulties. For example, our technique has been applied successfully to a crude unit system consisting of a 23-stage main fractionator and three side-cut strippers containing from three to four stages each. If I/O is of concern, then a standard LU decomposition could be used where the L and U matrices are overlayed, with U being an upper unit triangular matrix (i.e. unity on the main diagonal). As mentioned above, LU decomposition leads to precisely the same equations for p and q given by our method.

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ERRATA

In "Improving Distillation Column Design Using Thermodynamic Availability Analysis" by R. E. Fitzmorris and R. S. H. Mah [*AIChE J.*, **26**, 265 (1980)]
Equation (7a) should read

$$\beta_{hx} = q(1 - T_o/T_H) - q(1 - T_o/T_C) \quad (7a)$$

Equation (7c) should read

$$\beta_{hx} = (qT_o/T_C)(1 - T_C/T_o) + q(1 - T_o/T_H) \quad (7c)$$

Equation (8) should read

$$\beta_{hx} = T_o \int (dq/T_c) - T_o \int (dq/T_H) \quad (8)$$

Line 46, left column, p. 270 should read: "net work input as the vapor recompression . . .", not "net work input at the vapor recompression . . .".

Line 14, left column, p. 266 should read: "rate of irreversible entropy increase".

In "Oil Ganglion Dynamics During Immiscible Displacement: Model Formulation" by A. C. Payatakes, K. M. Ng and R. W. Flumerfelt [*AIChE J.*, **26**, 441 (1980)], Figure 11 appears sideways. The corrected version is shown below.

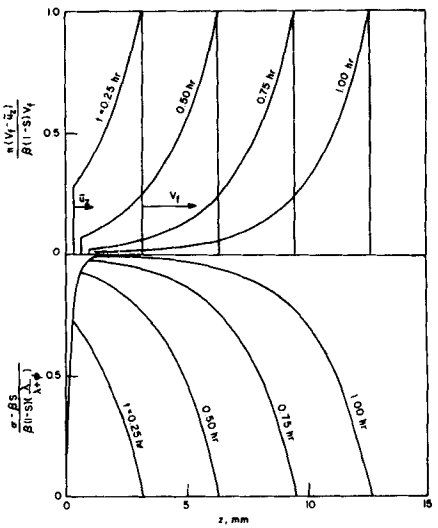

Figure 11. Traveling bulge of moving v ganglion concentration in the absence of coalescence. The corresponding stranded v ganglia concentration profile is also shown. Typical parameter values used in the calculation are: $V_f = 3.5$ μm/s, $\bar{u}_z = 0.35$ μm/s, $\lambda = 3$ mm^{-1}, $\phi = 2$ mm^{-1}.

1980 AIChE Membership Directory, American Institute of Chemical Engineers, New York (1980) 566 pp. This volume contains listings of officers of the Institute's Committees, Divisions and Local Sections, and alphabetical and geographical listings of members. Orders will be honored *only* from AIChE members. $10 (post-paid, prepaid only). Order from AIChE Publications Dept., 345 E. 47 St., New York, N.Y. 10017