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THE AUTHOR

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Optimal Decomposition of Process Networks

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The tearing or decomposition of recycle process networks is extended to include the enumeration of alternate cut sets or tear stream sets. The optimality criterion is the response to convergence acceleration in the quasi-Newton sense and an algorithm is proposed to select the optimum cut set adaptively as the recycle computation proceeds.

SCOPE

The object of this study is to reduce the computer time required to complete the steady state mass and energy balance calculations in a chemical process with recycle. In the modular simulation approach, the process model in the computer consists of a set of subroutines (operation modules) whose function is to calculate the properties of the physical output streams given the properties of the physical input streams and design parameters appropriate to each module, for example, the temperature in an isothermal flash module. The process model is thus composed of a network of streams and operation modules quite analogous to the usual flow sheet representation of the plant.

Completing the steady state simulation is a matter of identifying the recycle streams in the model and finding the properties of these streams, that is, temperature, pressure, enthalpy, flow rate and composition, which lead to stationary computation loops as the information flows are traced around the plant in the direction of physical flows from one module to its neighbor. One simple procedure is to guess the recycle stream properties and then allow the computer to iterate around process loops until recycle stream properties converge. This direct substitution approach yields the slowest approach to steady state. Considerable improvement can be achieved if the successive

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values of the recycle streams are extrapolated by fitting current and previous values to an equation, such as a straight-line, point-slope equation characteristic of the Newton-Raphson root finding technique.

The identification of recycle streams is not unique since any network may have alternate sets of recycle streams. Each set is called a *tear set* or *cut set* and is associated with a different sequence of operation module computations as the result of beginning at different points in the physical flow network. Computation begins at the tear streams with guessed values and the progress of the computation is checked when the tear streams finally reappear as operation module outputs. At this stage extrapolation or convergence acceleration may be applied and the sequence repeated.

If each tear stream set contains only one member, then all sets exhibit the same numerical behavior. However, if there are two or more streams in the alternate sets, then the numerical behavior of the decomposed network will differ from one set to another due to the differences in operation module sequences. The resulting computational procedures will respond more or less favorably to a convergence acceleration algorithm. The critical numerical properties of the computational loops are obtainable from the Jacobian matrices of the linearized decomposed network. These matrices are made up of the partial derivatives of each property in each tear stream appearing as an output with respect to each property in each tear stream appearing as an input. Such matrices may serve as multidimensional linear fits of successive tear stream values by which extrapolated values may be computed.

Most of the recent work in identifying tear streams is summarized in papers by Lee and Rudd (1966), Christensen and Rudd (1969), Forder and Hutchison (1969), Upadhye and Grens (1972), Barkley and Motard (1972), and Pho and Lapidus (1973). In some instances these authors will find a cut set that is minimal in the number of streams or, in other cases, minimal in the total number of significantly varying properties as an implication of computer efficiency. In this paper, the method of Barkley and Motard is extended to identify the important alternate cut sets with the help of a few simple rules that reduce the number of possible combinations.

The principle to be exploited in this work is an evaluation of the convergence properties of alternate cut sets while useful computations are performed using any one of the alternates. The alternate sets are identified first and loop calculations are begun with a likely candidate, generating the information required to build Jacobian matrices on all the sets. At suitable intervals the method may choose to switch cut set and sequence if a more rapid convergence is predicated for another set.

Thus, a method is proposed that is adaptive in searching out the optimal tear set in modular process simulation, assuring that the best performance will ultimately result, no matter that initial decisions are made as to the points of application of convergence acceleration in the process network.

CONCLUSIONS AND SIGNIFICANCE

As discussed in the Scope section, the choice of an optimum tear stream set in relation to convergence acceleration in achieving mass and energy balance in recycle process simulation appears to depend on the properties of the Jacobian matrices of the linearized process network. When the number of tear streams exceeds one, a theoretical analysis indicates that the matrix with the smallest maximum eigenvalue should identify the optimum tear set. Computing exact eigenvalues is itself a time-consuming task so an approximate criterion is proposed, namely, the sum of the squares of the diagonal elements of the various matrices. The matrix with the minimal sum indicates a possible optimum set and a switch is made while the computation is proceeding. This criterion only measures the sum of the squares of the eigenvalues.

Building the matrices themselves could be a problem; however, the quasi-Newton method of Broyden (1965) provides a dual framework for the adaptive search. It allows rapid estimation of Jacobians as well as convergence acceleration by multidimensional linear extrapolation using the same information. The estimation procedures uses only the successive input and output values of tear stream properties, whether actual tear streams or potential.

The method does find the optimum tear set, although the number of iterations is not always reduced when computations begin with a poor set. Further work on simple sensitivity criteria for switching cut sets may lead to a more rapid identification of the optimum and a more efficient exploitation of the theory. Of course, the results of a first computational pass at a network will guarantee maximum efficiency on subsequent case studies on the same network.

Recycle of material and energy in chemical process systems leads to the simultaneous solution of nonlinear algebraic equations when such systems are modeled mathematically. Two approaches to the modeling of these processes can be recognized, the first attempts to analyze all possible mathematical relationships both internal and external to the process unit, that is, the equation solving approach; and the second analyzes only the relationships external to the process units or modules, that is, the block-structured approach. In either case, a steady state solution of material and energy balances is sought, but the equation solving approach would appear to be more suitable to the design of a process and allows the imposition of constraints typical of and compatible with optimization problems.

The block-structured approach is more suitable for simulation studies (or design by case study) and generally implies that the identity of the output variables are known (the physical outputs of the process unit) and that the design variables have been preassigned by the programmer of the process module computer subroutines.

Our work concerns the block-structured approach. In solving nonlinear systems, one is led to iterative procedures either by repeated linearization or by various convergence acceleration techniques involving steepest-descent or Newton-type strategies or mixtures of the two. We include

repeated substitution or direct substitution as a special case of the latter. Part of the iterative procedure is the choice of tear variables or tear streams in the process network to which a convergence acceleration procedure is applied. The choice of the tear variables or streams is called *decomposition* and has as its objective the reduction of the original cyclic directed graph of the process to an acyclic graph by tearing or cutting a selected set of edges or nodes in the graph. The cut set is then the interface between the system model and the convergence procedure since the dimensionality of the problem has been reduced to just that of the cut or tear variables. To illustrate the notion of dimensionality, a process network containing a cyclical net of seven process streams could be viewed formally in a linearized model as a matrix of dimensionality M, where

$$M = \sum_{i=1}^{7} N_i$$

N_i = number of variables in stream i

and a one-step solution of the problem would be achieved by the inversion of an $M \times M$ matrix. On the other hand, a decomposition analysis might result in one cut stream j to tear the cyclic network completely and the same linearized model could be solved in one step by the inversion of an $N_j \times N_j$ matrix. In practice, the nonlinear system would be linearized repeatedly and iterated to final convergence.

We tend to favor the gradient or Newton-type strategies for their economy of computer time and memory requirements, but the notion of dimensionality reduction by decomposition is equally applicable.

OBJECTIVE FUNCTIONS IN OPTIMAL DECOMPOSITION

Previous work in the decomposition of block-structured networks (Barkley and Motard, 1972; Christensen and Rudd, 1969; Forder and Hutchison, 1969; Uphadye and Grens, 1972; Pho Lapidus, 1973) has concentrated on the tearing of a minimum of number of stream connections in the process or on the tearing of a minimum number of stream variables. Tearing stream variables implies that each stream connection is weighted according to the number of significant composition and other state variables associated with a stream. The objective function in these approaches is

$$\underset{\{I\}}{\text{Min}}\ \{J\} \quad \text{or} \quad \underset{\{Iw_i\}}{\text{Min}}\ \{Jw_j\}$$

either of which is presumed to minimize computation time by minimizing the cut set of streams $\{J\}$ over the set of all streams $\{I\}$ or cut set of stream variables $\{Jw_j\}$ where each cut stream is weighted by its significant state variables w_j. Neither criterion is sufficiently descriptive of the efficiency of solution achieved by decomposition, and the weighted stream approach suffers from the additional disadvantage that proper weighting functions may not be readily known by a user of a general purpose simulation package.

A more proper definition of an optimal decomposition objective function may be arrived at by considering that the real measure of computational efficiency is the rate of convergence of the decomposed network. Since it is presumed that a convergence acceleration algorithm will be interfaced to the cut set whether these be streams, stream variables, or, indeed, equation solving variables, then a suitable objective function must take into account the response of a specific convergence algorithm to particular sets of cut variables. This objective function cannot be generalized, but past work suggests, by analogy to linear

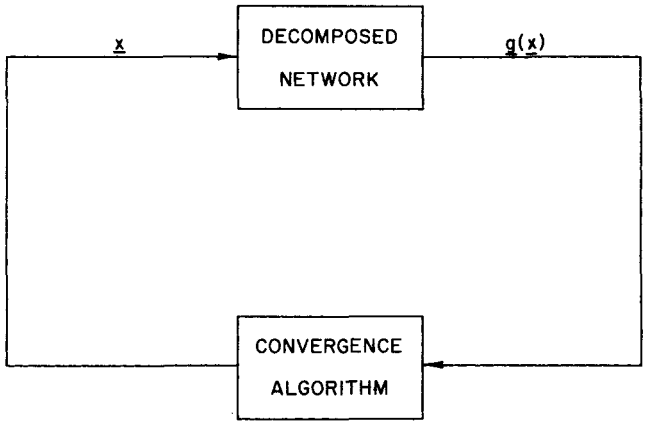

Fig. 1. General cyclic network.

systems behavior under a direct substitution discipline, that the sensitivity of the computational network to the cut variables should be minimized. While convergence and stability theorems for Newton-like methods are difficult to apply, the first-order Newton process involves a local linearization of the systems and, as such, the Jacobian matrix of the computation network with respect to the cut variables is in fact the sensitivity matrix and should have eigenvalues that are less than one in magnitude and a largest eigenvalue that is as small as possible.

To illustrate the application of sensitivity concepts, Figure 1 represents a typical iterative procedure on a decomposed network. Since the appropriate streams have been cut to introduce the convergence algorithm, the procedure is tantamount to the solution of the system

$$\mathbf{g}(\mathbf{x}) = \mathbf{x} \tag{1}$$

where $\mathbf{x}$ is the vector of cut stream variables.

Expanding $\mathbf{g}(\mathbf{x})$ in a Taylor series,

$$\mathbf{g}(\mathbf{x}_{n+1}) = \mathbf{g}(\mathbf{x}_n) + \mathbf{J}(\mathbf{x}_{n+1} - \mathbf{x}_n) \tag{2}$$

where the subscripts refer to the iteration index and

$$\mathbf{J} = \frac{\partial \mathbf{g}}{\partial \mathbf{x}}$$

the Jacobian of the decomposed network. Equation (2) under a direct substitution algorithm

$$\mathbf{x}_{n+1} = \mathbf{g}(\mathbf{x}_n) \tag{3}$$

becomes

$$\mathbf{g}(\mathbf{x}_{n+1}) = \mathbf{J}^{n+1}(\mathbf{g}(\mathbf{x}_0) - \mathbf{x}_0) + \mathbf{g}(\mathbf{x}_n) \tag{4}$$

Obviously, Equation (4) achieves stationarity, namely, $\mathbf{g}(\mathbf{x}_{n+1}) = \mathbf{g}(\mathbf{x}_n)$, if

$$\lim_{n \to \infty} \mathbf{J}^{n+1} = \mathbf{0} \tag{5}$$

and the solution is nontrivial if $g(x_0) \neq x_0$. The necessary and sufficient condition for the limit to exist is that all eigenvalues of $\mathbf{J}$ be less than one in magnitude. It can be shown that convergence is faster the smaller is the maximum eigenvalue (Ralston, 1965). The adherence to the principle that physical outputs be computed from physical inputs (Rinard and Ripps, 1965) guarantees that the gains in the linearized process network matrix are all less than one and the asymptotic behavior actually experienced on the computer confirms that $g(x)$ is convex. The latter condition leads to the conclusion that $\mathbf{J}$ for such a procedure is positive definite and has all positive eigenvalues.

A Newton-Raphson convergence algorithm on the function

$$f(x) = g(x) - x = 0 \tag{6}$$

takes the form of Equation (7)

$$x_{n+1} = x_n + (\mathbf{I} - \mathbf{J})^{-1} (g(x_n) - x_n) \tag{7}$$

at each iteration step. Note that

$$\frac{\partial f}{\partial x} = \mathbf{J} - \mathbf{I} \tag{8}$$

The eigenvalues of $(\mathbf{I} - \mathbf{J})^{-1}$ are equal to $(1 - \lambda_i)^{-1}$ where the λ_i are the eigenvalues of J. The convergence of the Newton-Raphson method does not depend on the magnitude of the eigenvalues but rather on the accuracy of the estimate of J. If J is known exactly, then this method is quadratically convergent provided the function f is analytic and that $\mathbf{I} - \mathbf{J}$ is nonsingular.

Nevertheless, given a choice of alternative cut sets we wish to choose the set that minimizes the maximum eigenvalue of the sensitivity matrix J. This criterion is appealing since the sensitivity matrix will not be known exactly and the obvious default if the acceleration procedure gets into trouble is direct substitution. The objective function for this choice is

$$\underset{\{C_j\}}{\text{Min}} \{\lambda_{j\max}\} \tag{9}$$

where $\{\lambda_{j\max}\}$ is the set of maximum eigenvalues of the Jacobians obtained from the set of alternatives $\{C_j\}$.

The objective function proposed above is consistent with the work of Orbach and Crowe (1971) on acceleration convergence of decomposed networks. In their work, the dominant eigenvalue of the matrix J is recognized as controlling the rate of convergence and the method concentrates on identifying the dominant value(s) for extrapolation to the steady state. Our objective function seeks to minimize the dominant values among alternate cut sets.

ALTERNATE CUT SETS

In a previous paper (Barkley and Motard, 1972), we described a list processing technique based on graph concepts that allowed the identification of the minimum number of cut streams K in the cyclic network. We choose not to weight the streams since each stream is assumed to consist of the entire list of component species in the process.

While the alternate cut streams are members of the graph intervals containing the original cut set as header nodes, it is important to reduce the combinatorial space to be searched for alternative sets since the evaluation of the objective function imposes some penalty in time. A few elementary principles are in order. Starting with all combinations of K cut streams which will tear all cycles, where K is the size of the minimum cut set obtained by the application of our original algorithm, we seek some a priori bounding criteria which allow discarding many of the combinations. We wish to minimize the size of $\{C_j\}$.

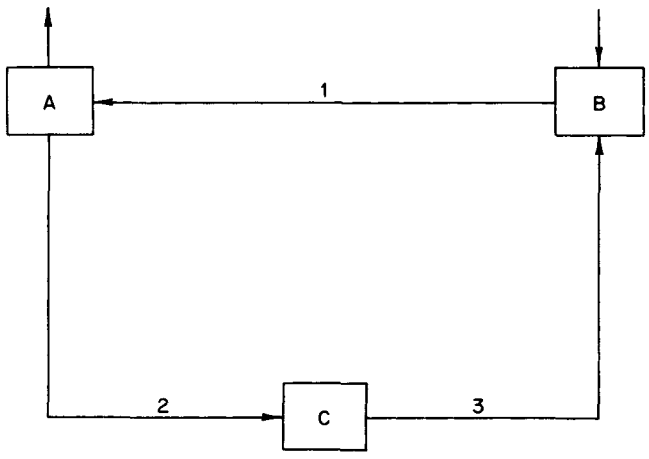

Fig. 2. A single loop process.

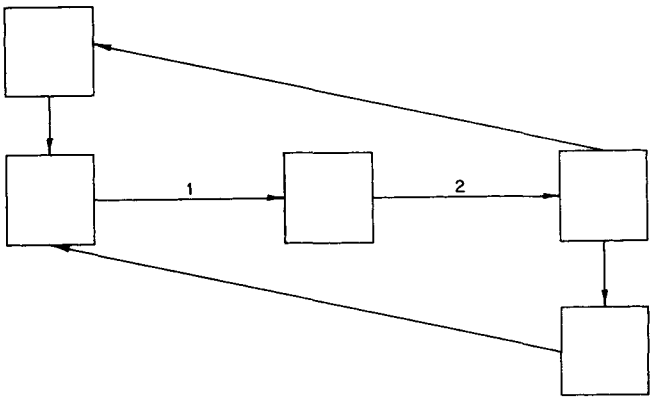

Fig. 3. Identical tear condition.

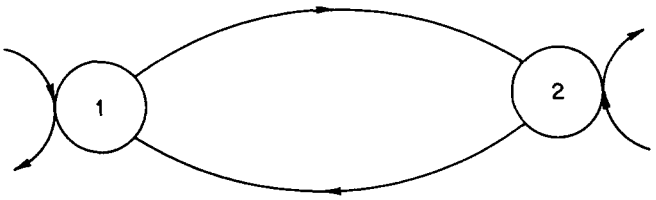

Fig. 4. Two-way edge pair.

The first bounding criterion relates to streams which appear in only one cycle of the network. Figure 2 is a general example of a single loop process which can be torn in one of three ways. Without detailing the simple algebra involved (Genna, 1973) it is obvious that the sensitivity matrix is identical no matter where the one-cycle process is torn since it is just the product of the sensitivity submatrices for process units A, B, and C taken in arbitrary order. Thus, streams which are members of only one cycle are all equivalent with regard to our criteria and may be reduced to one arbitrary stream.

The second bound relates to process streams which have only one successor or one precursor. These pairs can be reduced to a one stream alternative since the process sensitivity is the same for either the input or the output stream. Such a situation is shown in Figure 3 where streams 1 and 2 belong to two cycles, yet either one will generate the alternative sets.

The third bounding criterion relates to two-way edge stream pairs in the reduced flow graph of the network. At least one of the pair nodes must be a member of each alternate cut set. In Figure 4 either stream 1 or stream 2 must be a member of all alternate sets to keep K minimal.

Two examples of the application of the first three bounding criteria are taken from Cavett (1963) and Lee and Rudd (1966). In the first, shown in Figure 5, our decomposition algorithm finds $K = 2$ with streams 3 and 5 as the cut set.

Proceeding with the identification of alternatives, we find that streams 1 and 2 are members of only one loop or fit our second criterion. The same can be said of streams 6 and 7. The new network is shown in Figure 6.

Application of our third criterion reveals that streams 2 and 3 form a two edge pair and so do streams 5 and 7. No combinations with 4 and 8 would tear all cycles while

retaining $K = 2$. Of the four possible combinations left only three will tear all cycles: (3, 5), (3, 7), (2, 5)

The second example is shown in Figure 7.

The decomposition procedure again yields $K = 2$ with (8, 9) as the cut set. Applying the third criterion, the initial reduction of the graph yields node pairs (2, 8) and (5, 8). The residual combinations are (2, 8), (2, 5), (5, 8) and (8, 1), (8, 3)*, (8, 4), (8, 6)*, (8, 7), (8, 9), (8, 10)*. At this point we can appeal to a fourth bounding criterion, namely, that combinations at the level of K which involve immediate successors will not tear the graph. This eliminates the starred ( )* combinations. We are left with six possible alternates to (8, 9) which when tested directly for their ability to decompose the network result in five failures and one successful tear: (2, 5). Thus, this network has only two alternatives at the level, $K = 2$.

Further ad hoc criteria are possible. Since set (2, 5) are both inputs to the same unit, one might exploit the nature of this unit if in fact streams 2 and 5 are mixed directly in the unit. In that case the block should be divided into two serial blocks with the connecting stream being the mixture of 2 and 5. K is now reduced to one and all alternate sets are eliminated.

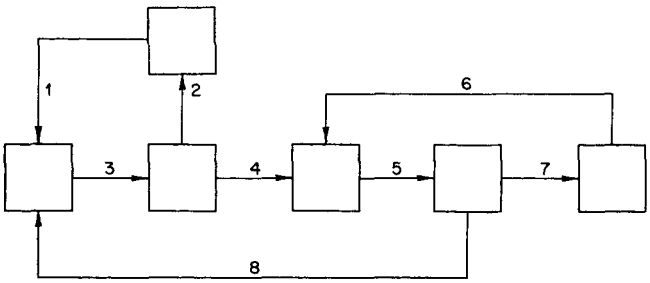

Fig. 5. Cavett's problem.

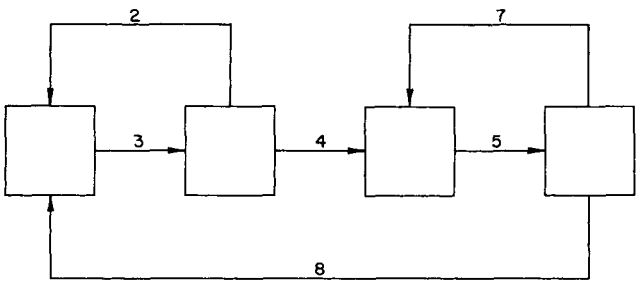

Fig. 6. Reduction of Figure 5.

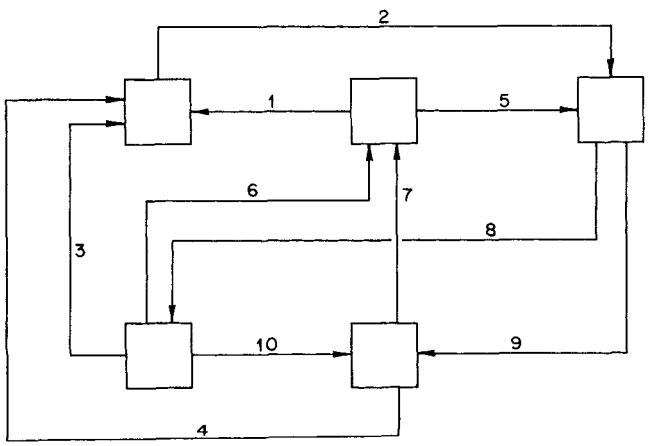

Fig. 7. Lee and Rudd problem.

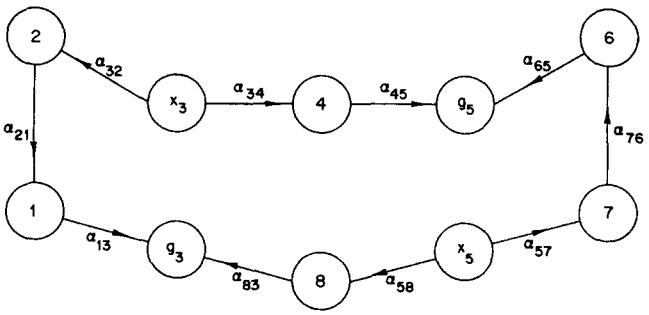

Fig. 8. A decomposition of Figure 6.

SENSITIVITY ANALYSIS

For decomposed networks with alternate cut sets, it is sometimes possible to make a priori judgments regarding the Jacobian or sensitivity matrix relative to the alternate cut sets. This allows an initial choice of cut sets based on the linearized system. With reference to the Cavett Problem, Figure 5, a flow graph (streams as nodes) is shown in Figure 8 with the split fractions α_{ij} representing the fraction of stream i transmitted to stream j. The α_{ij} of course are all equal to or less than unity. Where reactor blocks are involved the method of Rosen (1962) retains the generality of the split fraction concept. The cut nodes are divided into an output node g_i and an input node x_i, as shown in Figure 8 for cut set (3, 5). For cut set (3, 5) and one variable per stream the Jacobian is

$$\begin{bmatrix} \frac{\partial g_3}{\partial x_3} & \frac{\partial g_3}{\partial x_5} \\ \frac{\partial g_5}{\partial x_3} & \frac{\partial g_5}{\partial x_5} \end{bmatrix} = \begin{bmatrix} \alpha_{32}\alpha_{21}\alpha_{13} & \alpha_{58}\alpha_{83} \\ \alpha_{34}\alpha_{45} & \alpha_{57}\alpha_{76}\alpha_{65} \end{bmatrix} \tag{10}$$

Similarly, for cut sets (3, 7) and (2, 5) the matrices become

$$\begin{bmatrix} \alpha_{32}\alpha_{21}\alpha_{13} + \alpha_{34}\alpha_{45}\alpha_{58}\alpha_{83} & \alpha_{76}\alpha_{65}\alpha_{58}\alpha_{83} \\ \alpha_{34}\alpha_{45}\alpha_{57} & \alpha_{76}\alpha_{65}\alpha_{57} \end{bmatrix} \tag{10a}$$

$$\begin{bmatrix} \alpha_{21}\alpha_{13}\alpha_{32} & \alpha_{58}\alpha_{83}\alpha_{32} \\ \alpha_{21}\alpha_{13}\alpha_{34}\alpha_{45} & \alpha_{58}\alpha_{83}\alpha_{34}\alpha_{45} + \alpha_{57}\alpha_{76}\alpha_{65} \end{bmatrix} \tag{10b}$$

Since streams 3 and 5 are the outputs of simple mixing junctions, $\alpha_{13} = \alpha_{83} = \alpha_{65} = \alpha_{45} = 1$. This makes it somewhat easier to visualize the properties of the three matrices. Jacobians (3, 5), (3, 7), and (2, 5) become

$$\begin{bmatrix} \alpha_{32}\alpha_{21} & \alpha_{58} \\ \alpha_{34} & \alpha_{57}\alpha_{76} \end{bmatrix} \qquad \begin{bmatrix} \alpha_{31}\alpha_{21} + \alpha_{34}\alpha_{58} & \alpha_{58}\alpha_{76} \\ \alpha_{34}\alpha_{57} & \alpha_{57}\alpha_{76} \end{bmatrix}$$

and

$$\begin{bmatrix} \alpha_{21}\alpha_{34} & \alpha_{58}\alpha_{32} \\ \alpha_{21}\alpha_{34} & \alpha_{58}\alpha_{34} + \alpha_{57}\alpha_{76} \end{bmatrix} \tag{11}$$

where it is obvious that the second matrix is more diagonally dominant than the first, given $\alpha_{ij} < 1$. Diagonal dominance may be an advantage in itself since the quasi-Newton method that we will employ builds up the inverse Jacobian incrementally on each computation cycle in the network from an initial identity matrix. Both (3, 7) and (2, 5) would appear to be better initial choices for starting cut sets in the iteration of the material and energy balance to steady state. The proposed method attempts to improve the choice fo cut set adaptively as the iterative computations proceed.

ADAPTIVE CONVERGENCE ALGORITHM

Since the best cut set is the one whose Jacobian has minimum eigenvalues, the determination of which cut set to choose is made while useful computational work is progressing.

One chooses, by the methods described earlier, one of the $\{C_j\}$ to begin the convergence forcing of the network and then the properties of all Jacobian matrices for the $\{C_j\}$ are tested periodically to determine which cut set offers the best convergence properties. At any stage the system is accelerated by the quasi-Newton algorithm. The importance of minimizing the number of cut set choices by all available criteria cannot be overestimated since considerable work is involved in building and testing the sensitivity matrices.

Every network calculation generally begins with all internal streams initially zero. Only the external inputs to the network have been defined. The Jacobian for the selected initial cut set is the identity matrix (direct substitution). Then three direct substitution iterations are performed during which time the Broyden inverse Jacobian is being developed and the information required to build sensitivity matrices is being stored. This amounts to two vectors of the same length as the number of chemical species in the process per stream in the alternate cut sets per network iteration cycle. Two additional quasi-Newton steps are taken, and at the end of the fifth iteration a check of matrix eigenvalues can be made to evaluate alternate cut sets. If another cut set proves to be superior, the Broyden inverse Jacobian for this set is generated from the same information acquired for eigenvalue tests.

BROYDEN METHOD

The quasi-Newton method of Broyden (1965) (see also Rosen, 1966) avoids the computation of a new Jacobian matrix at each iteration step. Starting with an initial estimate of the inverse Jacobian, usually the identity matrix, the inverse is updated at each iteration step by secant approximations to the partial derivatives. As the approximated inverse approaches the true inverse, the quasi-Newton method experiences the quadratic convergence of the Newton method.

In applying the method within a block-structured simulation program, we have found it expedient to accelerate only the composition variables (moles/unit time) and not the temperatures of the streams which is the only other independent state variable. Pressures of streams are usually fixed by specification, and frequently temperatures are fixed at certain points in the process which means that forcing stream temperatures does not affect overall convergence to any detectable degree. Based on the cut set composition variables we want

$$g(x^k) - x^k = 0 = f(x^k) \tag{12}$$

where k is the iteration count. The quasi-Newton algorithm presumes that

$$d^k = x^{k+1} - x^k = \mathbf{H}^k f^k \tag{13}$$

where d is the direction and step size vector and $\mathbf{H}$ is an approximation to $(\mathbf{I} - \mathbf{J})^{-1}$, the inverse Jacobian of f. Updating $\mathbf{H}$ is obtained by the transformation:

$$\mathbf{H}^{k+1} = \mathbf{H}^k - \frac{[d^k + \mathbf{H}^k(f^{k+1} - f^k)]\, d^{kT}\mathbf{H}^k}{d^{kT}\mathbf{H}^k\,(f^{k+1} - f^k)} \tag{14}$$

Whenever it is necessary to use direct substitution H is updated by defining

$$d^k = g^k - x^k = f^k \tag{15}$$

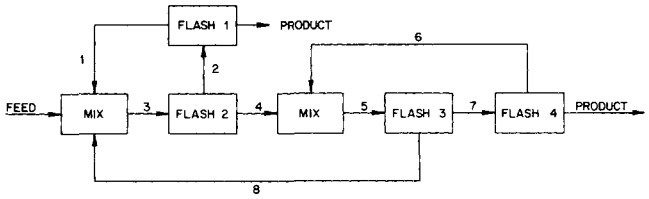

Fig. 9. Cavett's problem.

In all cases

$$x^{k+1} = x^k + d^k. \tag{16}$$

There are three circumstances when direct substitution must be employed: (1) at the beginning of the iteration process before an acceptable estimate of $\mathbf{H}$ is obtained ($k = 1, 2, 3$); (2) any time the denominator of Equation (14) approaches zero; (3) any time d_i changes sign on successive steps. These avoid problems due to the serial delay in obtaining a valid $\mathbf{H}$ and suppose that direct substitution is an infallible estimator of direction while the Newton method may or may not yield a good estimate of step size. Control of the x_i's to prevent negative values is also exercised.

The sensitivity matrices ($\mathbf{J}$) or estimates of $\mathbf{H}$ for alternate cut sets may be reconstructed at any time if one saves two vectors per stream per iteration over a span of a few steps, namely g^k and x^k for, say, three history steps. The iterative approximation to $\mathbf{J}$ is $\mathbf{B}$ (Broyden, 1965):

$$\mathbf{B}^{k+1} = \mathbf{B}^k + \frac{[(g^{k+1} - g^k) - \mathbf{B}^k d^k]\, d^{kT}}{d^{kT}d^k} \tag{17}$$

Since all streams not in the current cut set are being updated by direct substitution, only one vector needs to be saved at each history step ($x^{k+1} = g^k$ for streams not being accelerated).

Selecting a cut set with minimal eigenvalues is based on some norm of $\mathbf{J}$. In our case, while we expect all eigenvalues to be positive, we cannot discount the fact that at specific iterations they may not be, due to the round off errors and other numerical problems due to the approximations used. We therefore elect to choose the cut set with the minimum

$$\text{trace } (\mathbf{B}^2) = \sum_{i=1}^{n} \lambda_i^2 \tag{18}$$

Having obtained $\mathbf{B}$ by Equation (17), n vector inner products will yield the elements of the trace.

EXAMPLE 1

For Cavett's Problem (1963), the structure is as shown in Figure 9.

The simulation runs were made with K-values computed from stream properties using the CHESS (Motard) simulation program. Direct substitution converges in 27 iterations (0.1% tolerance). The results for cut sets (3, 5) is 13 iterations, cut set (3, 7) 12 iterations and cut set (2, 5) 10 iterations. Other attempts to find ad hoc combinations of cut sets at the level of one, two, or three streams all yielded convergence at intermediate levels of fourteen to seventeen iterations. The quasi-Newton convergence algorithm was applied on 16 components of two cut streams simultaneously, that is, a 32 × 32 inverse Jacobian matrix was generated. A plot of the convergence of a key component (*i*-butane) is given in Figure 10 for cut stream sets (2, 5) and (3, 5).

The eigenvalues of the $\mathbf{H}$ matrix at convergence were

Table 1. λ_H, Eigenvalues of H at Convergence

Cut set	(2,5)	(3,7)	(3,5)
λ_i (max.)	0.5815	0.6162	0.7153
*1.	2.3896	2.6062	3.5137
2.	(1.0494, .0381)	(1.0255, .1439)	1.2656
3.	(1.0494, −.0381)	(1.0255, −.1439)	0.6970
4.	1.0126	1.1372	0.8437
5.	0.9961	.9523	(.9433, .0655)
6.	1.0014	1.0309	(.9433, −.0655)
7.	1.0004	1.0115	(1.0186, .0048)
8.	1.0003	0.9978	(1.0186, −.0048)
9.	1.0003	1.0010	1.0072
10-32.		Remaining λ_H very close to 1.0	

* λ_H yielding largest λ_i.
( ) complex value.

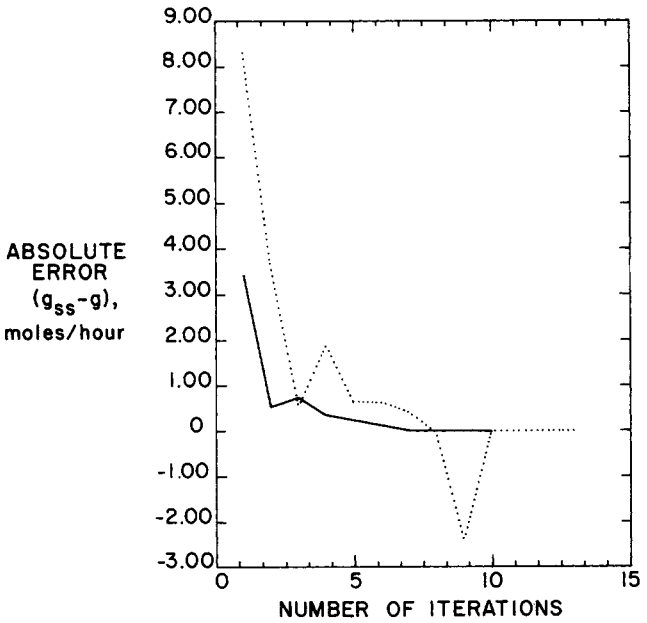

Fig. 10. Convergence of *I*-butane in Stream 5.

computed using the EISPACK system (Argonne National Laboratory, Applied Mathematics Division). The maximum eigenvalues λ_i for **J** correspond to the maximum eigenvalues for **H**

$$\lambda_{imax} = (\lambda_{Hmax} - 1)/\lambda_{Hmax} \qquad (19)$$

and are given with the EISPACK results for λ_H in Table 1. The λ_i(max.) values support the theory and qualitatively support the differences in observed iterations to convergence. It is also obvious that some of the λ_i are complex and some are negative, but these effects are small and do not vitiate our original premises based on direct substitution behavior since they probably arise from the dynamics of the quasi-Newton procedure. It is also apparent that there is not much variable interaction in the example process since so many of the eigenvalues are close to one. A profile of λ_i(max.) for each cut-set is shown in Figure 11.

The adaptive algorithm was next applied to each of the three cut sets as a starting choice. The sensitivity analysis switched cut sets as indicated in Table 2. The results are just as conclusive that (2, 5) is the optimal choice although the selectivity appears to be more delicate than originally anticipated. A better criterion than the square of the trace of B may be needed to improve selectivity at earlier stages of iteration.

Table 2. Behavior of Adaptive Convergence Algorithm for Example 1

Initial cut set	Change of cut set	Convergence	Without adaptation
(2,5)	—	10 iterations	10
(3,7)	(3,5) at iteration 6 (2,5) at iteration 12	13 iterations	12
(3,5)	(2,5) at iteration 9 (3,5) at iteration 12 (2,5) at iteration 18	18 iterations	13
Direct substitution			27

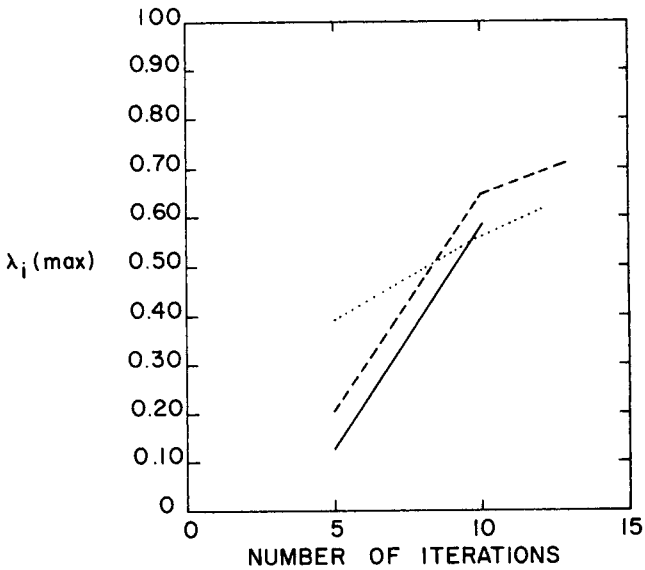

Fig. 11. Maximum eigenvalue profiles, Example 1.

EXAMPLE 2

The same problem was solved using a fixed set of *K*-values given by Cavett. The results are shown in Table 3 with the maximum eigenvalue profiles for the nonadaptive cases shown in Figure 12. Again there is some qualitative support for the theory although the comparison is less conclusive. Cut set (2, 5) is the winner, nevertheless. Generally, the maximum eigenvalues are larger for the second example and exceed one in some instances, but the be-

havior of cut set (3, 7) is unusual suggesting a serious lack of monotone behavior. For the latter case the algorithm attempts to interpolate too often and defaults to direct substitution frequently.

DISCUSSION

The behavior of quasi-Newton convergence acceleration and direct substitution in simulated process recycle networks is shown to be dependent on the maximum eigenvalues of the Jacobian matrices resulting from different tear stream combinations. The result for direct substitution in the different contexts agrees with the theory. The rate of convergence of the Newton-Raphson method does not depend on the eigenvalues of the linearized system, but the quasi-Newton form of the method responds favorably to choosing the tear stream set with minimal maximum eigenvalue. Two reasons are suggested for the latter behavior: (1) the tear set with the best properties generates a Jacobian with more diagonal dominance that the other alternatives and, (2) the above property improves the ability of the Broyden method to estimate an inverse Jacobian more accurately. The second characteristic is what improves the performance of the quasi-Newton method.

Adaptively searching for the optimum tear set while the computation proceeds is successful in locating the best set but does not result in faster convergence if one begins with a poor choice. A more precise criterion for choosing the best tear set (without resorting to the actual calculation of eigenvalues) than the one used here is needed. Of course, the results of a first simulation pass on a recycle network will improve performance of subsequent case studies on the same network.

TABLE 3. BEHAVIOR OF ADAPTIVE CONVERGENCE ALGORITHM FOR EXAMPLE 2

Initial cut set	Change of cut set	Convergence	Without adaptation
(2,5)	—	15 iterations	15
(3,5)	(3,7) at iteration 6 (2,5) at iteration 12	24 iterations	22
(3,7)	(2,5) at iteration 9 (3,7) at iteration 12 (2,5) at iteration 15	25 iterations	26

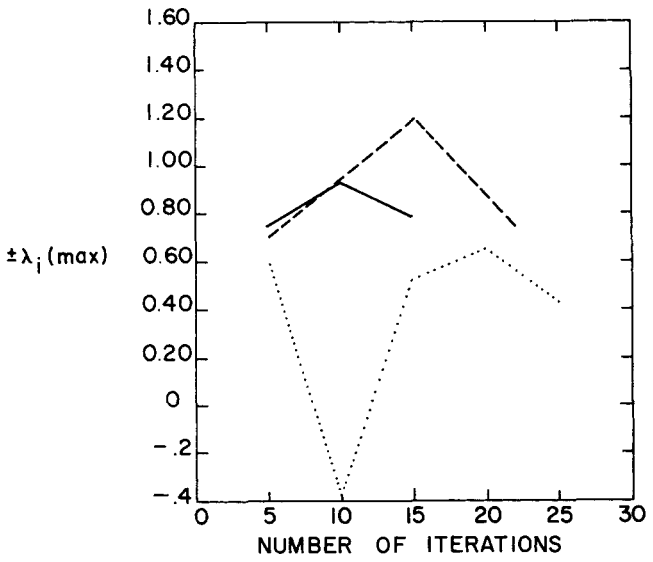

Fig. 12. Maximum eigenvalue profiles, Example 2.

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NOTATION

$\mathbf{B}$ = Broyden approximation of $\mathbf{J}$
C_j = $\{C_j\}$, the set of alternate cut sets
$\mathbf{d}$ = vector-valued difference, $\mathbf{x}^{k+1} - \mathbf{x}^k$
$\mathbf{f}$ = vector-valued function $\equiv \mathbf{o}$
$\mathbf{g}$ = vector-valued function $\equiv \mathbf{x}$
$\mathbf{H}$ = Broyden approximate inverse of $\mathbf{I} - \mathbf{J}$
M, N = dimensions
I = $\{I\}$, the set of all streams
$\mathbf{I}$ = identity matrix
J = $\{J\}$, one cut set of streams
$\mathbf{J}$ = Jacobian matrix
K = minimum number of cut streams to tear a network
k = superscript, iteration number
n = subscript, iteration number
n = superscript, power n
T = superscript, transpose
w_i, w_j = weights of variables in $\{I\}$ and $\{J\}$
$\mathbf{x}$ = vector of variables in cut stream set

Greek Letters

α_{ij} = fraction of stream i transmitted to stream j
λ_i, λ_j = eigenvalues of Jacobian matrix of $\mathbf{g}$
λ_H = eigenvalues of matrix $\mathbf{H}$
$\mathbf{o}$ = null vector

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