Structural Analysis and Solution of Systems of Algebraic Design Equations

A new method for expressing the structure of a system of equations is developed using a type of occurrence matrix entitled the *functionality matrix*. The functionality matrix indicates not only the occurrence of variables in equations but also the functional form in which they occur. Since the difficulty of solving an equation for a variable is related to its functional form, analysis of the functionality matrix provides explicit information on the difficulty of solution of the equation.

A methodology for the solution of design problems by digital computers is described. This methodology operates on the functionality matrix which describes the set of design equations. Algorithms using this methodology interact and guide the designer in an efficient selection of design variables and redundant equations. Once design variables and redundant equations are selected, a computational method is presented for ordering and solving the equations.

N. L. BOOK and
W. F. RAMIREZ

Department of Chemical Engineering
University of Colorado
Boulder, CO 80309

SCOPE

Design equations are predominantly algebraic, often nonlinear, and commonly sparse in that each equation contains only a few of the system variables. The major difference between a simulation study and a design study is the parameters specified. The input, output, or combinations of input and output specifications may be known in a design study. Specified parameters may change from one solution to another. Equipment parameters and unspecified input and output parameters are the result of the calculations. All input and equipment parameters must be specified in a simulation study and the output parameters are calculated. The structure for simulation studies is set. This allows simulation studies to be formulated into a modular approach (Motard et al., 1975).

Analysis of the characteristics of design problems demonstrates that a need exists for a methodology for analysis of systems of design equations. This methodology must be oriented at the equation, not modular, level since the calculation path is not fixed for a design problem. This publication reports the development of a method for analyzing systems of equations which characterize design problems. Techniques for selecting design variables and redundant equations are given and methods for obtaining the solution to the system of equations efficiently are presented.

CONCLUSIONS AND SIGNIFICANCE

A new, flexible methodology is developed for the structural analysis and solution of large systems of algebraic equations. Application is made for the solution of design problems. The development which links the structural analysis with problem solution is the functionality matrix. The functionality matrix allows for the structural analysis and solution of systems of unordered, underconstrained systems of equations which may contain redundant equations.

Efficiency in the solution of large systems of algebraic problems is gained by the use of the solution methodology presented in this work. No ordering of the equations or logic is necessary in programming the solution of a system of equations.

STRUCTURAL ANALYSIS

Structural analysis is the study of the interrelationships and interactions among the various components that form a system. The goal is the attainment of the simplest, most efficient calculation path between the components that form the system. In simulation calculations, the components are modules representing the process equipment, the interactions are process streams, and the calculation sequence is determined by the direction of flow in the process streams. In design calculations, the components are the mathematical equations, the interactions are between the variables that appear in the equations, and the calculational path is undirected.

The crux of the ordering problem for process simulation arises when all modules have at least one precursor. This indicates the presence of a recycle stream. The initial algorithms developed by Sargent and Westerberg (1964), Lee and Rudd (1966), and Christensen and Rudd (1969) sought to minimize either the number of process streams or the total number of variables in the cut set (the variables requiring initial guesses for initiation of an iterative solution technique). This recognized the fact that convergence problems tend to increase with the size of the cut set. Upadhye and Grens (1972) altered the basic algorithms to include a weighting factor for each variable in a stream. Convergence of simulation calculations are generally more stable than design calculations since they proceed along the path of the physical stream flows. Shacham and Motard (1974) show that direct substitution must converge for every physically realizable simulation system with initial guesses close enough to the actual solution. The convergence rate, however, may be slow. The directed flows of the process flowsheet provide the foundation for the high degree of refinement achieved for structural analysis of simulation problems.

Structuring design calculations varies from structuring simula-

Present address of N. L. Book: Department of Chemical Engineering, University of Missouri, Rolla MO.

TABLE 1. FUNCTIONAL FORMS OF EQUATIONS

Form Designation	Functional Form	Equation Form
A	Linear	$C_1^*x_1 + f(x) = 0$
B	Product	$C_1^*x_1^*x_2 + f(x) = 0$
D	Triple Product	$C_1^*x_1^*x_2^*x_3 + f(x) = 0$
H	Exponential	$C_1^*C_2x_1 + f(x) = 0$
I	Hyperbolic Sine	$C_1^* \sinh(x_1) + f(x) = 0$
J	Hyperbolic Cosine	$C_1^* \cosh(x_1) + f(x) = 0$
K	Hyperbolic Tangent	$C_1^* \tanh(x_1) + f(x) = 0$
L	Natural Logarithm	$C_1^* \ln(x_1) + f(x) = 0$
M	Common Logarithm	$C_1^* \log(x_1) + f(x) = 0$
N	Cubic Form	$C_1^*x_1^3 + f(x) = 0$
P	Power Form	$C_1^*x_1C_2 + f(x) = 0$
Q	Quadratic Form	$C_1^*x_1^2 + C_2^*x_1 + f(x) = 0$
R	Fourth Order Form	$C_1^*x_1^4 + f(x) = 0$
S	Second Order Form	$C_1^*x_1^2 + f(x) = 0$
T	Sine	$C_1^* \sin(x_1) + f(x) = 0$
U	Cosine	$C_1^* \cos(x_1) + f(x) = 0$
V	Tangent	$C_1^* \tan(x_1) + f(x) = 0$

E\V	x_1	x_2	x_3	x_4	f_i
1		A	A		2
2		A	A	S	3
3	A		S		2
r_j	1	2	3	1	

(a)

E\V	x_2	x_3	x_4	x_1	f_i
1	A	A			
2	A	A	S		
3		S		A	
r_j	2	3	1	1	

(b)

E\V	x_2	x_3	x_4	x_1	f_i
1	A	A			
2					
3		S		A	
r_j					

(c)

E\V	x_3	x_2	x_4	f_i
3	S			1
1	A	A		2
2	A	A	S	3
r_j	3	2	1	

(d)

E\V	x_3	x_4	x_1	f_i
1	A			1
2	A	S		2
3	S		A	2
r_j	3	1	1	

(e)

E\V	x_2	x_4	x_1	f_i
1	A			1
2	A	S		2
3			A	1
r_j	2	1	1	

(f)

E\V	x_2	x_3	x_1	f_i
1	A	A		2
2	A	A		2
3		S	A	2
r_j	2	3	1	

(g)

Figure 1. Functional effects on solution sequences.

tion calculations in two significant ways. The first is the undirected format of design equations. In the analysis of design equations, an order must be assigned to the equations and the equation must be assigned a variable for which to be solved. This assignment is the admissible output set of Steward (1965). The second variation lies in the inability of simulation calculations to circumvent a module. Design calculations often have numerous parallel paths, not all of which must be taken. Each of the parallel paths must be analyzed to determine the path which provides the minimum calculational difficulty.

Parallel paths in design problems arise from the existence of the degrees of freedom in design variables and redundant equations. Steward (1965) and Himmelblau (1967) studied the assignment of admissible output sets for systems of algebraic equations which contained no design variables or redundant equations. The first attempt to develop a mathematical basis for the selection of design variables was the bipartite graph structure of Lee, Christensen and Rudd (1966). The algorithm given in terms of the more convenient occurrence matrix is presented in Rudd and Watson (1968). The algorithm fails for systems of equations with persistent iteration. Christensen (1970) developed an algorithm which handles persistent iteration. The algorithm of Stadtherr et al. (1974) tends to yield nested, implicit iterative loops, both of which are to be avoided for iterative calculations using direct substitution. Ramirez and Vestal (1972) present algorithms which are constructed in two phases. The first phase selects the design variables for the system and determines the minimum number of iterative variables for the system. The second phase selects iterative variables so as to obtain explicit iterative loops if possible. Algorithms by Westerberg and Edie (1971) and Edie and Westerberg (1971) use the maximum eigenvalue principle to select design variables. One of the major limitations of all of these algorithms is that they produce a single combination of design and iterative variables. Book and Ramirez (1976) developed methods of expressing all solution sequences which are acyclic for systems of equations without persistent iteration and all solution sequences with a minimum number of iterative variables in systems of equations with persistent iteration. Friedman and Ramirez (1973) show that convergence of explicit iterative loops by the methods of direct substitution is dominated by the order of solution of the equations in the loop. Convergence by direct substitution will occur on the reverse path if the forward path diverges and the reverse path exists.

FUNCTIONALITY MATRIX

The prime requisite of a method for expressing the structure of a system of algebraic equations is that the structure be explicitly expressed. The occurrence matrix is not an explicit representation in that it only expresses the occurrence structure of a system of equations. To remove this deficiency, a new type of occurrence matrix was developed called the functionality matrix. In order to express the functional form of an equation the different functional forms in which a variable can appear in equations must be defined. Table 1 gives the various functional forms which were considered. In Table 1, C_i are constants and $f(x)$ can be a function of all the other system variables except the explicit variables. The functional forms of Table 1 are those which predominate in algebraic design equations. By using the state variable approach almost any equation can be algebraically altered to fit such forms. The functionality matrix is, therefore, a special occurrence matrix which expresses both equation structure and functionality.

The example functional matrix of Figure 1a demonstrates the effects of the functional forms of equations. The functionality matrix (Figure 1a) is a representation of the following equations:

$$C_1x_2 + C_2x_3 + C_3 = 0 \tag{1}$$

$$C_4x_2 + C_5x_3 + C_6x_4^2 + C_7 = 0 \tag{2}$$

$$C_8x_1 + C_9x_3^2 + C_{10} = 0 \tag{3}$$

If the constants are $C_1 = 1$, $C_2 = 1$, $C_3 = -5$, $C_4 = -2$, $C_5 = 1$, $C_6 = 3$, $C_7 = -2$, $C_8 = 2$, $C_9 = 1$, $C_{10} = -17$, the desired solution is $x_1 = 4$, $x_2 = 2$, $x_3 = 3$, and $x_4 = 1$.

The matrix of Figure 1b is the rearranged matrix (Book and Ramirez, 1976) of Figure 1a and the matrix of Figure 1c is the solution mapping matrix (Book and Ramirez, 1976) of the rearranged matrix. The problem does not contain persistent iteration. The solution mapping matrix indicates that the selection of x_1, x_2 or x_3 will reduce the rearranged matrix such that it has an acyclic solution sequence.

The matrix of Figure 1d is the acyclic solution sequence for the case when x_1 is chosen as the design variable. The solution sequence encounters some difficulty in the solution of Eq. 3 for variable x_3 since multiple roots of ± 3 are available as solutions to the quadratic equation. A physical distinction must be made between these two roots, if the design problem has a single, real solution. It is sometimes quite difficult to distinquish between the two roots unless further calculations are made with both roots. Continuing with the solution sequence and solving Eq. 1 for x_2 gives $x_2 = 2$ or 8. This has increased the difficulty in that there are two solutions each associated with one of the two solutions for x_3. The final step in the solution sequence is to solve Eq. 2 for x_4. This gives values of $x_4 = \pm 1$ or $\pm 4i$. It has now been determined that $x_3 = -3$ and $x_2 = 8$ corresponds to an imaginary root. Also, physical distinction must be made between the ± 1 values for x_4. Clearly this computational path leads to difficulties.

The matrix associated with Figure 1e corresponds to the selection of x_2 as the design variable. The square term in Eq. 3 presents no difficulty since it does not enter as an output variable. A physical distinction must, however, be employed to select the correct root for variable x_4. The functionality matrix of Figure 1e would be considered an easier solution sequence than the sequence represented by the functionality matrix of Figure 1d due to the elimination of carrying two solutions through the calculations.

The solution sequence represented by the functionality matrix of Figure 1f (x_3 is the design variable) is equal in difficulty structurally to that of Figure 1e. This is due to the fact that only one multiple root appears as an output variable.

The selection of x_4 as a design variable does not yield an acyclic solution sequence. This is indicated by the solution mapping matrix (Figure 1c). However, proper arrangement of the rows and columns of the matrix results in the functionality matrix of Figure 1g. This matrix describes the solution of two linear equations (Eqs. 1 and 2) in two unknowns (x_2 and x_3) followed by the solution of Eq. 3 which is linear in variable x_1. Due to the fact that the solution of simultaneous linear equations are easily obtained, the functionality matrix of Figure 1g is considered as the simplest to obtain for machine computation. The acyclic calculations involving multiple root functionals actually increases the complexity in obtaining the solution.

From the information contained in the normal solution mapping matrix, solution sequences can only be differentiated as to acyclicity or cyclicity with a minimum of tear elements. By including information on the functional form of the equation to be solved, the "optimality" of a solution sequence can be analyzed in much greater depth. Even to the point, as the example has shown, of sacrificing acyclicity.

OBJECTIVE FUNCTION

The explicit representation of a system of equations contained in the functionality matrix allows differentiation among numerous types of available solution strategies. This allows algorithms to be developed for defining suitable objective functions for decomposition. A suitable objective function should yield a maximum solution efficiency considering available solution methods. For example, if equations are to be solved by hand, direct substitution with a single iterative variable (explicit or implicit) is often an excellent method. Likewise, multiple roots can be easily carried along in hand calcualtions. However, for implementation on digital computers, general methods for the solution of implicit iterative loops are not well established. With machine computation, methods which employ matrix manipulations are desirable.

For machine computation of algebraic equations describing design problems, the following heuristic objective function was selected:

1. Assign arbitrarily an acyclic output element to a single equation if the solution for the output element is single valued. If not possible, go to step 2.
2. For a linear set of equations, assign arbitrarily output variables to that set. If not possible, go to step 3.
3. Assign arbitrarily an acyclic output element to a single equation with multiple roots. If not possible, go to step 4.
4. Assign arbitrarily the minimum number of iterative variables to equations which contain those variables.

The Equation Ordering and Variable Group Algorithms of Book and Ramirez (1976) were altered to use this heuristic objective function. Figures 2 and 3 present the algorithms. A prototype computer program (Book, 1976) which has been developed to implement these algorithms does not seek linear simultaneous equations. However, if the algorithms are implemented by hand, the designer can easily detect the occurrence of linear simultaneous equations. The algorithms (Figures 2 and 3) result in a rearranged functionality matrix for the system of equations. Platform variables, output variables, step equations, subgroups, and the matrix partitions are apparent (Book and Ramirez, 1976).

The Equation Ordering Algorithm searches the variable degrees of freedom for values of one. The existence of a one indicates that an acyclic assignment can be made. The entry is located, and the row is eliminated if the functional designation indicates a single-valued functional. If the function designation indicates a multiple-valued function, the column location is stored in MULCOL. If all the variable degrees of freedom are searched and no single-valued acyclic assignment is made, a set of linear simultaneous equations are desired (Level 2 of the objective function). If a linear simultaneous assignment cannot be made, MULCOL is checked to see if an acyclic multiple-root assignment can be made (Level 3 of the objective function). As the variable degrees of freedom are searched, the column with the minimum value greater than one is stored in MINCOL. This variable indicates the equations to be eliminated in assigning the minimum number of iterative variables. Hierarchy pointers store the location of step equation in systems with persistent iteration.

The Variable Group Algorithm searches the equation degrees of freedom. If a value of one is encountered, the equations are "shuffled" to move the equation up into the subgroup being formed. The column (variable) containing the entry is then eliminated. While in a cyclic equation set, no "shuffling" is done. This avoids moving additional equations into an iterative loop. When no value of one is encountered for the equation degrees of freedom, a new set of platform variables (a new cyclic equation set) is formed by eliminating the columns containing entries in the topmost row. Subgroup pointers store the location of the platform variables.

NUMERICAL ANALYSIS METHODS

Previously developed methods of structual analysis were not directly linked to the solution phase of the problem. The structural information of the ordering of equations and admissible output sets were results from the structural analysis routines. It then remained for the designer to make the necessary algebraic manipulations, incorporate the required solution methods, and program the solution strategy. This is no longer the case. The functionality matrix allows reconstruction of an equation to within a set of constants. When these constants are specified, the equation can be solved efficiently. Therefore, the development of the functionality matrix leads to a formulation for the analysis and solution of unordered sets of algebraic equations. Initially, the set of algebraic equations to be solved are algebraically manipulated to fit the acceptable forms of Table 1. In our prototype implementation, each functional form was expressed as a function subroutine of the form

$$f(x) = 0. \tag{4}$$

The functionality matrix yields information describing these equations to within a set of constants. The constants are evaluated by making selected guesses for the values of the variables that ap-

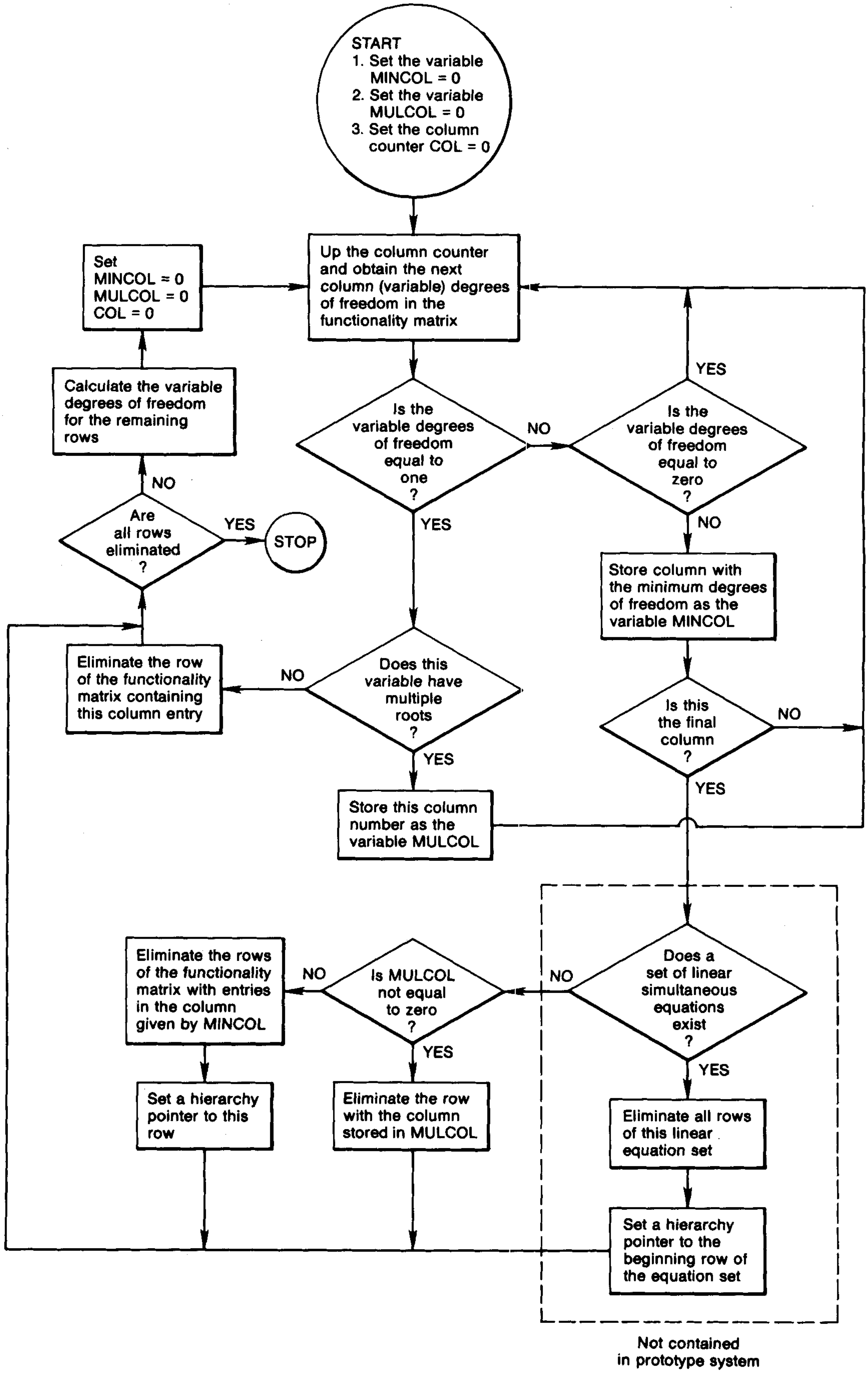

Figure 2. Equation ordering algorithm.

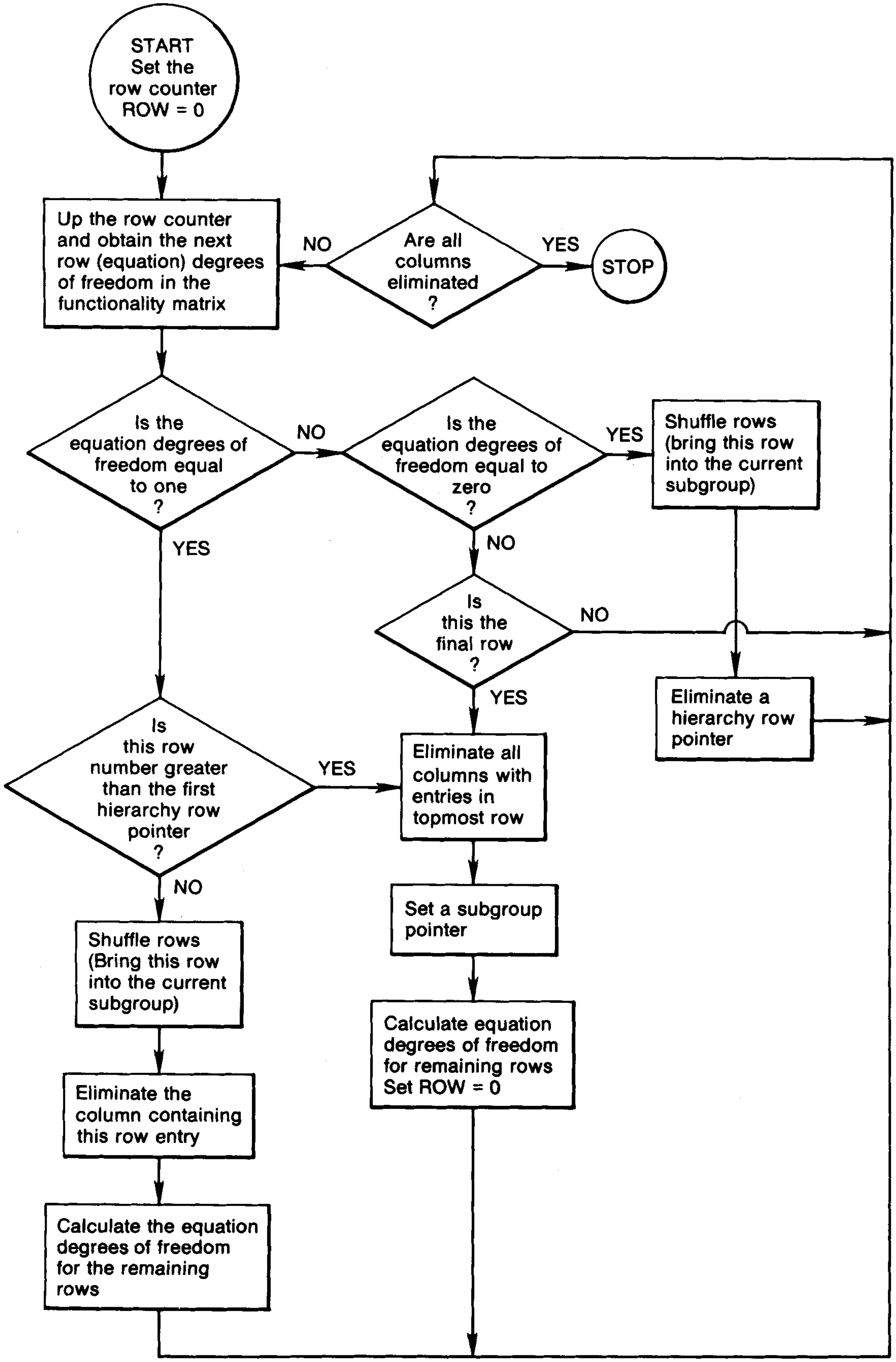

Figure 3. Variable group algorithm.

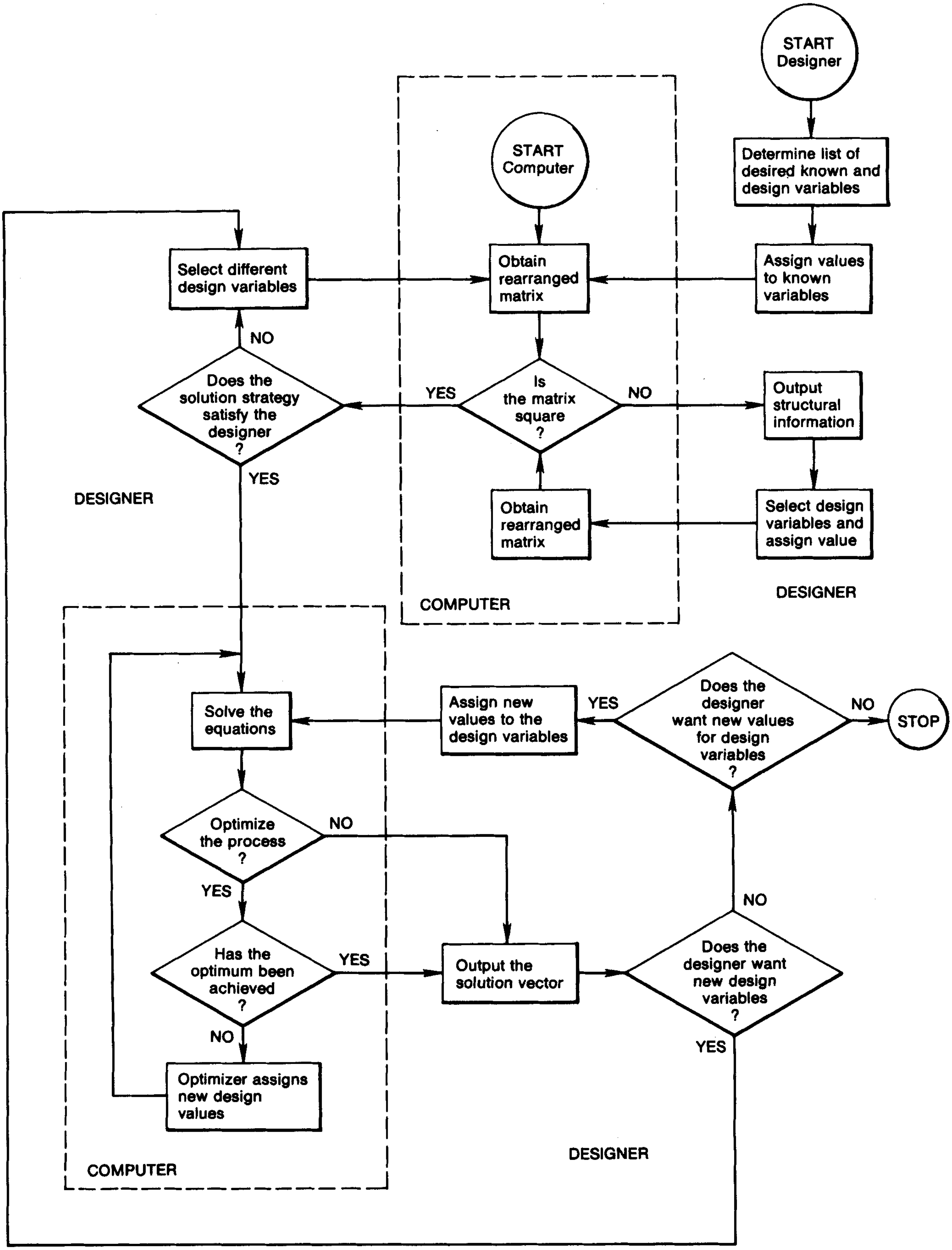

Figure 4. Methodology for structural analysis and solution of large systems of equations.

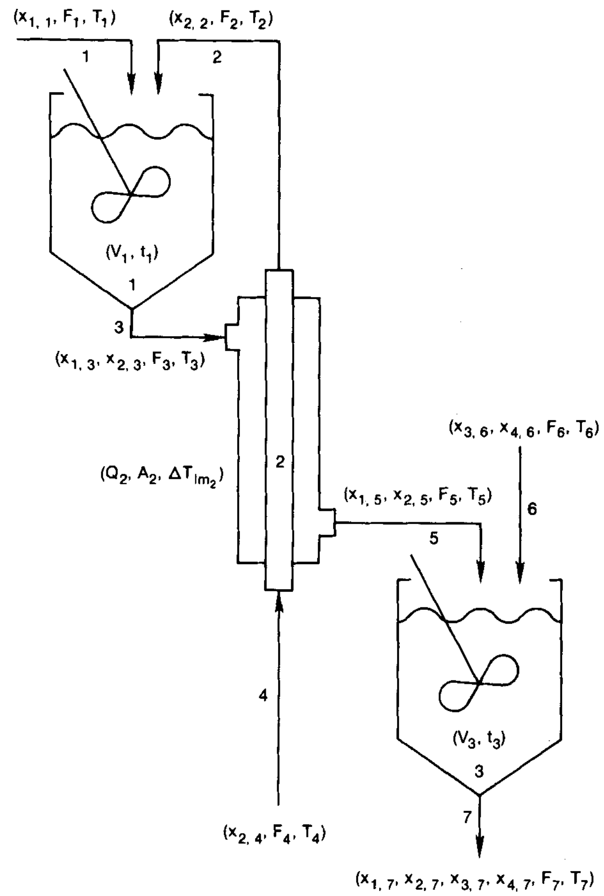

Figure 5. Mixer-exchanger-mixer system.

pear in the equations. The function subroutine returns a value of the variable as well as an error estimate. Subroutines contained in Book (1976) have been developed which accomplish the logic necessary to solve both acyclic and cyclic functionals. For nonlinear cyclic functionals, algorithms using the Newton-Raphson method, and the Broyden (1965) method have been developed.

METHODOLOGY FOR SOLUTION OF DESIGN PROBLEMS

A complete methodology for structual analysis and solution which uses the functionality matrix is given in Figure 4. This methodology naturally lends itself to an interactive mode of operation where the structural information in the rearranged matrix is output to the designer who chooses design variables and assigns numerical values to them. The selection of design variables is done efficiently if an initial list of design variables is constructed and the rearranged matrix is obtained. If the solution strategy obtained is not difficult, structural analysis is not necessary and the solution to the equation set is sought. If the solution strategy is more difficult than desired, the rearranged matrix for the equations with the known variables removed represents the starting point for the structural analysis. The structural information contained in the rearranged functionality matrix guides and aids in the choice of design variables.

Minimum Difficulty Strategy

The rearranged functionality matrix provides the designer with the expected difficulty of the simplest strategy available. Hierarchy information indicates the presence and size of persistent iteration loops. Persistent iteration loops can be analyzed for the possibility of linear simultaneous equations.

TABLE 2. EQUATIONS FOR MIXER-EXCHANGER-MIXER SYSTEM

Material Balance Equations

Mole Fraction Equations

1. $x_{1,1} - 1 = 0$
2. $x_{2,2} - 1 = 0$
3. $x_{1,3} + x_{2,3} - 1 = 0$
4. $x_{2,4} - 1 = 0$
5. $x_{1,5} + x_{2,5} - 1 = 0$
6. $x_{3,6} + x_{4,6} - 1 = 0$
7. $x_{1,7} + x_{2,7} + x_{3,7} + x_{4,7} - 1 = 0$

Flow Balance Equations

8. $F_1 + F_2 - F_3 = 0$
9. $F_2 - F_4 = 0$
10. $F_3 - F_5 = 0$
11. $F_5 + F_6 - F_7 = 0$

Component Balance Equations

12. $x^*_{1,1}F_1 - y_1 = 0$
13. $x^*_{1,3}F_3 - y_1 = 0$
14. $x^*_{1,5}F_5 - y_1 = 0$
15. $x^*_{1,7}F_7 - y_1 = 0$
16. $x^*_{2,2}F_2 - y_2 = 0$
17. $x^*_{2,3}F_3 - y_2 = 0$
18. $x^*_{2,4}F_4 - y_2 = 0$
19. $x^*_{2,5}F_5 - y_2 = 0$
20. $x^*_{2,7}F_7 - y_2 = 0$
21. $x^*_{3,6}F_6 - y_3 = 0$
22. $x^*_{3,7}F_7 - y_3 = 0$
23. $x^*_{4,6}F_6 - y_4 = 0$
24. $x^*_{4,7}F_7 - y_4 = 0$

Energy Balance Equations

25. $F_1 * T_1 - z_1 = 0$
26. $F_2 * T_2 - z_2 = 0$
27. $F_3 * T_3 - z_3 = 0$
28. $F_4 * T_4 - z_4 = 0$
29. $F_5 * T_5 - z_5 = 0$
30. $F_6 * T_6 - z_6 = 0$
31. $F_7 * T_7 - z_7 = 0$
32. $C_1 * z_1 + C_2 * z_2 - C_3 * z_3 = 0$
33. $C_4 * z_4 - Q_2 - C_2 * z_2 = 0$
34. $C_3 * z_3 + Q_2 - C_5 * z_5 = 0$
35. $C_5 * z_5 + C_6 * z_6 - C_7 * z_7 = 0$

Equipment Specification Equations

36. $V_1 - (F_3 * t_1)/\rho_3 = 0$
37. $Q_2 - U_2 * A_2 \Delta T_{lm_2} = 0$
38. $w_1 + T_3 - T_2 = 0$
39. $w_2 + T_5 - T_4 = 0$
40. $w_2 * w_3 - w_1 = 0$
41. $w_4 - ln\,(w_3) = 0$
42. $w_4 * \Delta T_{lm_2} + w_2 - w_1 = 0$
43. $V_3 - (F_7 * t_3)/\rho_7 = 0$

Capital Cost Estimation Equations

44. $\log(S_1) - 0.515 * \log(v_1) - 3.354 = 0$	v_1 (m^3)
45. $v_1 - V_1 = 0$	V_1 (m^3)
46. $\log(S_2) - 0.699 * \log(A_2) - 2.414 = 0$	A_2 (m^2)
47. $\log(S_3) - 0.515 + \log(v_3) - 3.354 = 0$	v_3 (m^3)
48. $v_3 - V_3 = 0$	V_3 (m^2)
49. $S - S_1 - S_2 - S_3 = 0$	S (1969 \$)

Platform Variables

Platform variables are known to be contained in desirable design variable combinations. The selection of platform variables is therefore preferred. If multiple-root functionals appear with simple-valued functionals in platform variable sets, it is useful to select the multiple-root functional variables as design variables.

Subgroup Interaction Matrix

Some important information is contained in the subgroup interaction matrix for the rearranged functionality matrix. The

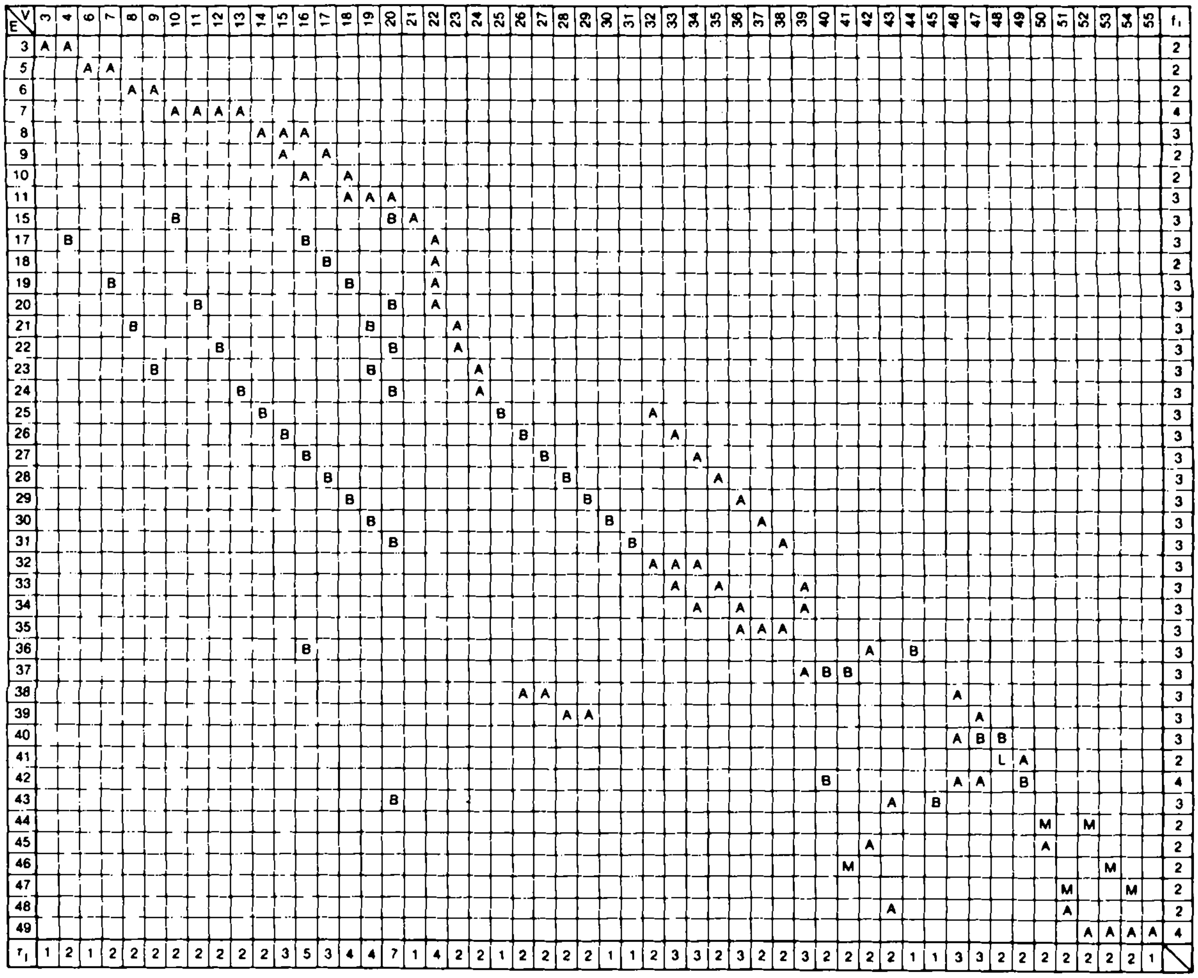

Figure 6. Original functionality matrix of mixer-exchanger-mixer system with degree one and redundant equations removed.

concept of equation dependence is not used to remove any of the equations in the rearranged functionality matrix as is done to construct a solution mapping matrix (Book and Ramirez, 1976). This subgroup interaction matrix is formed from partitions of the rearranged matrix containing all equations. Two types of subgroups can be defined.

Predecessor Independent Subgroups

A subgroup is predecessor independent if only a main diagonal entry appears in the row of the subgroup interaction matrix representing the equations associated with the subgroup. For a digraph representation, this indicates no edges entering the node (Subgroup 1 is predecessor independent in Figure 10). Predecessor independent subgroups are important because the selection of design variables associated with the subgroup allows for the solution of the equations associated with the subgroup. Subgroup 1 is always predecessor independent. Selection of design variables in predecessor independent subgroups leads to reduction in the size of the system of equations.

Successor Independent Subgroups

A subgroup is successor independent only if a main diagonal entry appears in the column of the subgroup interaction matrix representing the subgroup. For a digraph representation, this indicates that the node has no edges pointed toward another node (Subgroups 4, 7 and 9 are successor independent in Figure 9). For the rearranged functionality matrix, a successor independent subgroup indicates that *no* solution is possible without selecting design variables from among the subgroup variables.

TABLE 3. VARIABLE ASSIGNMENTS

Desig. Var.	Number	Desig. Var.	Number	Desig. Var.	Number
$x_{1,1}$	1	y_1	21	A_2	41
$x_{2,2}$	2	y_2	22	V_1	42
$x_{1,3}$	3	y_3	23	V_3	43
$x_{2,3}$	4	y_4	24	t_1	44
$x_{2,4}$	5	T_1	25	t_3	45
$x_{1,5}$	6	T_2	26	w_1	46
$x_{2,5}$	7	T_3	27	w_2	47
$x_{3,6}$	8	T_4	28	w_3	48
$x_{4,6}$	9	T_5	29	w_4	49
$x_{1,7}$	10	T_6	30	v_1	50
$x_{2,7}$	11	T_7	31	v_3	51
$x_{3,7}$	12	z_1	32	S_1	52
$x_{4,7}$	13	z_2	33	S_2	53
F_1	14	z_3	34	S_3	54
F_2	15	z_4	35	S	55
F_3	16	z_5	36		
F_4	17	z_6	37		
F_5	18	z_7	38		
F_6	19	Q_2	39		
F_7	20	ΔT_{1m_2}	40		

The difficulty caused by the selection of any design variable in a subgroup is found by trial and error. The final subgroup is always successor independent. Successor independent subgroups indicate subgroups in which design variables are trapped. The designer must select design variables in successor independent subgroups.

The designer analyzes successor independent subgroup variables

E \ V	9	8	19	18	16	14	32	27	26	33	34	39	36	29	47	37	38	48	49	40	41	42	50	52	53	55	7	6	4	31	3	f_i
6	A	A																														2
23	B		B																													2
21		B	B																													2
11			A	A																												2
10				A	A																											2
8					A	A																										2
25						A	A																									2
38								A	A																							2
26									A	A																						2
32							A			A	A																					3
27					B			B			A																					3
33										A		A																				2
34											A	A	A																			3
29				B									A	B																		3
39														A	A																	2
30			A													A																2
35													A			A	A															3
40															B			B														2
41																		L	A													2
42															A				B	B												3
37												A								B	B											3
36					A																	A										2
45																						A	A									2
44																							M	M								2
46																					M				M							2
49																								A	A	A						3
19				B																							B					2
5																											A	A				2
17					B																								B			2
31																	A													A		2
3																													A		A	2
r_j	2	2	4	4	5	2	2	2	2	3	3	3	3	2	3	2	2	2	2	2	2	2	2	2	2	1	2	1	2	1	1	

Figure 7. Rearranged matrix with known and preliminary design variables removed.

and selects a partial set of design variables and another rearranged matrix is obtained. If the solution strategy is suitable to the designer, the new successor independent subgroups are analyzed. If the solution strategy is not suitable, the designer must find replacements for variables currently in the design variable set.

Once a satisfactory design variable combination is determined, the computer is allowed to solve the equations using the various solution routines available. Optimization methods can be used if desired.

MIXER-EXCHANGER-MIXER DESIGN

The production of methylamines from methanol and ammonia is economically affected by the ratio of the demands of the three products (monoethylamine, dimethylamine and trimethylamine). The recycle of trimethylamine will reduce the production of dimethylamine and trimethylamine relative to the production of monomethylamine. Similarly, the dilution of the reaction mixture with water will result in a relative increase in the production of monoethylamine. A mixer-heat exchanger-mixer portion of a methylamine plant is a proposed capital investment which would allow the relative production of the methylamines to be varied to meet changes in demand.

A detailed schematic for the mixer-exchanger-mixer system is shown in Figure 5. Trimethylamine recycle enters in stream 4, is cooled in the heat exchanger, and is mixed with water from stream 1 in mixer 1. The trimethylamine-water mixture is used as the cold side fluid in the heat exchanger and is then mixed with the ammonia-methanol stream from the gas absorber in mixer 3. The mixture leaving mixer 3 is the reaction mixture which feeds into the preheater of the existing plant. A preliminary estimate of the cost of installing the mixer-heat exchanger-mixer system is desired. A generic mixer-exchanger-mixed problem has been studied by Ramirez and Vestal (1972).

The installation is modeled by the 49 equations presented in Table 2 all of which fit an acceptable form from Table 1. There are four redundant material balance equations. Each of the 55 variables is assigned a number for convenience (Table 3). The functionality matrix for the system of equations is shown in Figure 6 (redundant equations have been removed as will be later demonstrated). The installation of the mixer-exchanger-mixer system into the existing plant tends to specify certain of the process variables. The temperatures of the entering streams (T_1 T_4 and T_6) are known. Likewise it is desired to produce a flow rate and composition of the exit stream which meets the proper specifications. Hence, values are set for variables F_7, $x_{1,7}$, $x_{2,7}$, $x_{3,7}$ and $x_{4,7}$. Only three of the four exit mole fractions are independent and may be

E\V	16	18	20	19	15	14	17	22	11	7	6	4	3	24	13	9	8	23	12	10	21	35	39	33	26	28	34	32	36	25	27	29	46	47	48	49	40	41	53	37	30	38	31	44	42	50	52	43	45	51	54	55	f_i
10	A	A																																																			2
11		A	A	A																																																	3
8	A				A	A																																															3
9					A		A																																														2
18							A	A																																													2
20			B					A	B																																												3
19		B						A		B																																											3
5										A	A																																										2
17	B							A				B																																									3
3												A	A																																								2
24			B											A	B																																						3
23				B										A		B																																					3
6																A	A																																				2
21				B													B	A																																			3
22			B															A	B																																		3
7									A						A				A	A																																	4
15			B																	B	A																																3
33																						A	A	A																													3
26					B																			A	B																												3
28							B															A				B																											3
32																								A			A	A																									3
34																							A				A		A																								3
25						B																						A		B																							3
27	B																										A				B																						3
29		B																											A			B																					3
38																									A						A		A																				3
39																										A						A		A																			3
40																																	A	B	B																		3
41																																			L	A																	2
42																																	A	A		B	B																4
37																							A														B	B															3
46																																						M	M														2
30				B																																				A	B												3
35																													A											A		A											3
31			B																																							A	B										3
36	B																																											B	A								3
45																																													A	A							2
44																																														M	M						2
43			B																																													A	B				3
48																																																A		A			2
47																																																		M	M		2
49																																							A								A				A	A	4
r_j	5	4	7	4	3	2	3	4	2	2	1	2	1	2	2	2	2	2	2	2	1	2	3	3	2	2	3	2	3	1	2	2	3	3	2	2	2	2	2	2	1	2	1	1	2	2	2	2	1	2	2	1	

Figure 8. Rearranged matrix of mixer-exchanger-mixer with ten degrees of freedom.

specified as known variables. Therefore, of the ten degrees of freedom, seven are essentially specified as known variables via the problem. With seven known variables, three additional variables are required as design variables. The residence times for the two mixers (t_1 and t_2) and the cold end temperature difference of the heat exchanger (w_1) were preliminarily selected as possible design variables. These variables are not necessarily the best design variables for solution simplicity but are ones for which the designer can best assign reasonable values. Engineering experience, flow sheet analysis, and knowledge of the process mathematical model are used to construct the preliminary set of design variables, and are chosen whenever possible in the structural analysis. The preliminary set of design variables could contain any number of variables and does not have to exactly constrain the system.

Three rearranged matrices can be quickly obtained which indicate the need for and advantages gained by structural analysis. The first rearranged matrix is obtained with the known variables and the best set of design variables removed. If the solution sequence indicated in the rearranged functionality matrix is not difficult, there is no need for structural analysis if the preliminary design variables resulted in a constrained system of equations. The methodology of Figure 4 would then pass directly to the solution phase.

The rearranged functionality matrix for the mixer-exchanger-mixer system with the known and preliminary design variables removed is shown in Figure 7. Equations 12, 13, 14 and 16 were the redundant equations removed from the problem specification. The rearranged matrix contains a set of three nonlinear simultaneous equations and a set of four linear simultaneous equations. Equations 38, 26, 32 and 27 are linear even though Eq. 27 contains a product form since variable 18 will have been previously solved (Eq. 10) making Eq. 27 linear in variable 27. This solution strategy is not very difficult, however, for the purposes of this example was deemed too difficult and a simpler strategy was sought.

A second rearranged matrix was therefore obtained with the preliminary design variables (t_1, t_3 and w_1) not removed from the equation set. This second rearranged functionality matrix indicates the increased difficulty due to the preliminary design variable set. The results of this rearranged matrix still contained the set of three nonlinear simultaneous equations. Hence the three preliminary design variable set is not the cause for the nonlinear equation set.

A third rearranged functionality matrix when neither the known or design variables have been removed is shown in Figure 8. The matrix indicates that acyclic solutions are possible. This system has ten degrees of freedom. This rearranged functionality matrix has nine subgroups. A digraph representation of the subgroup interaction matrix is shown in Figure 9 along with a listing of the platform and output variables in each of the subgroups. Subgroups 4, 7 and 9 are successor independent and each has one design variable associated with the subgroup. Variables t_3, t_6 and $x_{4,7}$ were selected to serve as design variables to satisfy the requirements of these subgroups. All three are platform variables indicating that an acyclic strategy results with their selection. An additional platform variable, t_1, was also selected since it appears in the preliminary set of design variables. The variable F_7 which is part of the known variable set could be chosen at this time but was left for later selection.

With these four variables removed a new rearranged functionality matrix was obtained. One subgroup was successor independent and the minimum difficulty solution sequence available is acyclic. Neither of the platform variables appear in the list of

KNOWN VARIABLES

$x_{1,7}$ $x_{2,7}$ $x_{3,7}$ $x_{4,7}$ T_4 T_6 T_1 F_7

BEST PRELIMINARY DESIGN VARIABLES

t_1 t_3 w_1

SUBGROUP	PLATFORM VARIABLES	OUTPUT VARIABLES
1	F_3 F_5	
2	F_7 F_6	
3	F_2 F_1	F_4 y_2 $x_{2,7}$ $x_{2,5}$ $x_{1,5}$ $x_{2,3}$ $x_{1,3}$
4	y_4 $x_{4,7}$	$x_{4,6}$ $x_{3,6}$ y_3 $x_{3,7}$ $x_{1,7}$ y_1
5	z_4 Q_2 z_2	T_2 T_4
6	z_3 z_1	z_5 T_1 T_3 T_5 w_1 w_2 w_3 w_4 ΔT_{lm} A_2 S_2
7	z_6 T_6	z_7 T_7
8	t_1 V_1	v_1 S_1
9	V_3 t_3	v_3 S_3 S

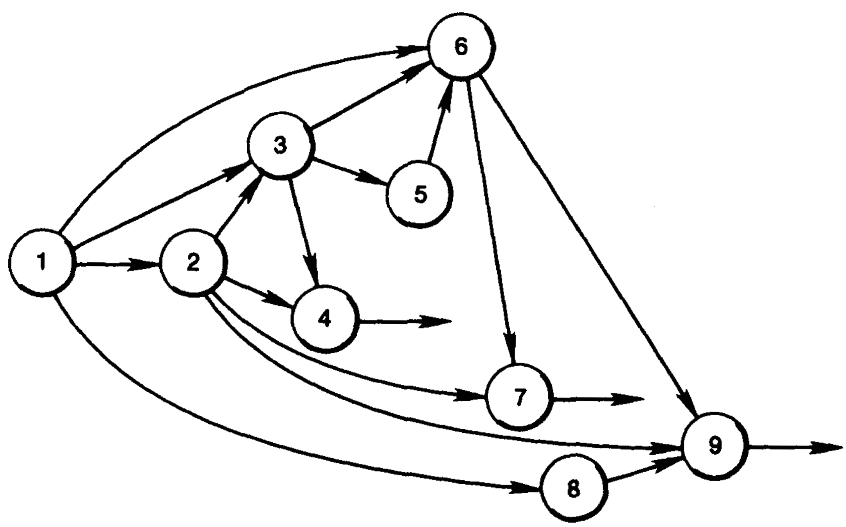

Figure 9. Digraph of subgroup interactions of rearranged matrix of figure 10.

known or preliminary design variables, therefore one of the output variables of this subgroup was chosen as a design variable (T_4). Since variable T_4 is an output and not a platform variable, an acyclic solution sequence is not guaranteed. Another rearranged matrix was then obtained and it showed that T_4 did allow for an acyclic solution sequence. From the digraph of the subgroup interaction matrix, the next variable T_1 was selected from a successor independent subgroup.

At this point, the resulting interaction subgroup digraph is shown in Figure 10. The only output variable in the preliminary set of known and desired design variables contained in successor independent subgroup 4 is w_1. The selection of w_1 was made and another rearranged matrix obtained. Persistent iteration was indicated in a set of four linear simultaneous equations. This does not represent a difficult solution strategy and w_1 would normally be retained. However, the goal of the structural analysis for this problem is an acyclic strategy. Therefore w_1 was replaced by another output variable of subgroup 4, namely T_2. The resultant rearranged matrix

CHOSEN VARIABLES

$x_{4,7}$ T_6 t_1 t_3 T_4 T_1

KNOWN VARIABLES

$x_{1,7}$ $x_{2,7}$ $x_{3,7}$ F_7

BEST PRELIMINARY DESIGN VARIABLES

w_1

SUBGROUP	PLATFORM VARIABLES	OUTPUT VARIABLES
1	$x_{3,6}$ $x_{4,6}$	
2	F_6 y_4	F_7 F_5 y_3 $x_{3,7}$ F_3 V_1 V_3 v_3 S_3 v_1 z_6 S_1
3	F_2 F_1	F_4 z_1 z_4 y_2 $x_{2,7}$ $x_{1,7}$ y_1 $x_{2,5}$ $x_{1,5}$ $x_{2,3}$ $x_{1,3}$
4	z_2 z_3	Q_2 z_5 T_2 T_3 T_5 z_7 T_7 w_2 w_1 w_3 w_4 ΔT_{lm} A_2 S_2 S

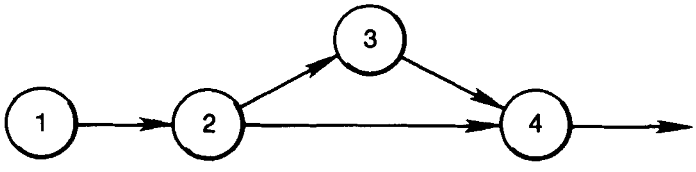

Figure 10. Digraph of subgroup interaction matrix with $x_{4,7}$, T_6, t_1, t_3, T_4, and T_1 removed.

was without persistent iteration. Variable $x_{1,7}$ was selected from the output variables of the successor independent subgroup and the solution strategy was still acyclic. A final subgroup interaction digraph indicated variable F_7 as a platform variable and was selected at this time. Variables $x_{2,7}$ and $x_{3,7}$ which were assumed as known during the original design appear in a successor independent subgroup. Only one degree of freedom remains so the two mole fractions are not independent. The selection of either results in a set of three nonlinear simultaneous equations. In order to obtain an acyclic strategy, a variable must be chosen to replace the mole fractions in the product stream. Variable $x_{3,6}$ was selected since it was a platform variable and an acyclic solution is assured. The problem was easily solved following this acyclic solution strategy.

REDUNDANT EQUATIONS

The optimal selection of redundant equations to remove in a set of algebraic equations using structural analysis has not been previously addressed. Each set of equations must have the redundant equations removed before solution. The selection of which equations to remove can alter the difficulty of the resulting solution strategies. Sets of redundant equations can be classified into the two groups of 1) overspecified sets and 2) specified or unspecified sets. In overspecified sets the number of design variables is less than the number of redundant equations. In specified or underspecified sets, the number of design variables is equal to or greater than the number of redundant equations.

The existence of overspecified sets of redundant equations are easily identified by the occurrence matrix representation. The set of redundant equations will have an occurrence matrix with more rows than columns. It is an absolute indication of redundant equations in properly posed design problems.

For specified and underspecified sets of redundant equations, all sets of redundant equations appear as a set of equations which contain persistent iteration. The converse, however, is not true. The selection of redundant equations for this case, therefore, requires that the designer know the equations in the redundant sets and the number of redundant sets. An alternative strategy would be the

E \ V	5	2	1	9	8	24	19	23	13	20	12	18	16	10	11	22	7	6	21	4	3	17	15	14	f_i
4	A																								1
2		A																							1
1			A																						1
6				A	A																				2
23				B		A	B																		3
21					B		B	A																	3
24						A			B	B															3
22								A		B	B														3
11							A			A		A													3
10												A	A												2
7									A		A			A	A										4
20										B					B	A									3
19												B				A	B								3
5																	A	A							2
15										B				B					A						3
14												B						B	A						3
17													B			A				B					3
13													B						A		B				3
3																				A	A				2
18	B															A						B			3
9																						A	A		2
16		B														A							B		3
8													A										A	A	3
12			B																A					B	3
τ_j	2	2	2	2	2	2	3	2	2	5	2	4	4	2	2	5	2	2	4	2	2	2	3	2	

Figure 11. Rearranged matrix of material balance equations in mixer-exchanger-mixer problem.

checking of the determinant of the Jacobian matrix for all groups of equations with persistent iteration.

The objectives for selecting which redundant equations are:
1) to obtain a set of acyclic equations,
2) to eliminate nonlinear sets of simultaneous equations and
3) to eliminate elements in the largest groups of simultaneous linear equations.

The rearranged functionality matrix is useful in selecting the best redundant equations to remove. Sets of redundant equations always contain persistent iteration and therefore appear as step equations.

The rearranged functionality matrix for the 24 material balance equations of the mixer-exchanger-mixer design problem are shown in Figure 11. There are four redundant equations. The persistent iteration can be removed from the material balance equations by eliminating one of each of the four pairs of step equations.

Set	*Redundant Equation*
1	15 or 14
2	13 or 3
3	9 or 16
4	8 or 12

The number of redundant equations exactly equals the number of iterative variables in this rearranged matrix. The four sets of step equations must, therefore, contain independent equations in the four redundant sets. Any of the 16 combinations of four redundant equations will make ths problem acyclic.

ACKNOWLEDGMENT

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NOTATION

$x_{i,j}$ = mole fraction of component i in stream j
F_j = molar flow rate of stream j(gmol/h)
y_i = molar flow rate of component i(gmol/h)
T_j = temperature of stream j (°C)
z_j = state variable substitution for $F_j * T_j$
Q_k = heat transferred in unit k (cal/h)
A_k = heat transfer area for unit k (m^2)
V_k = volume of unit k (m^3)
t_k = residence time for unit k (h^{-1})
w_1 = state variable substitution
v_k = volume of unit k (m^3)
S_k = cost of unit k (1969 $)
S = total cost of installation (1969 $)
C_j = molar heat capacity of stream j (cal/gmol·°C)
U_k = overall heat transfer coefficient of unit k (cal/h·m^2·°C)
f_i = row frequency of row i
ρ_k = molar density of fluid in unit k (gmol/cm^3)
τ_j = column frequency of column j
ΔT_{1m_k} = log mean temperature difference for unit k (°C)

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Coalescence Time for a Small Drop or Bubble at a Fluid-Fluid Interface

JING-DEN CHEN,
PIL SOO HAHN and
J. C. SLATTERY

Department of Chemical Engineering
Northwestern University
Evanston, IL 60201

When a small drop or bubble is driven through a liquid phase to a fluid-fluid interface, a thin liquid film which forms between them drains, until an instability forms and coalescence occurs. Lin and Slattery (1982b) developed a hydrodynamic theory for the first portion of this coalescence process: the drainage of the thin liquid film which occurs while it is sufficiently thick that the effects of London-van der Waals forces and electrostatic forces can be ignored. Here we extend their theory to include the effects of the London-van der Waals forces. To simplify the analysis, we follow the suggestion of Buevich and Lipkina (1975, 1978) in developing an expression for the rate of thinning at the rim or barrier ring of the draining film. A linear stability analysis permits us to determine the coalescence time or the elapsed time between the formation of a dimpled film and its rupture at the rim.

For comparison, this same linear stability analysis is applied to the thinning equations developed by MacKay and Mason (1963) for the plane parallel disc model and by Hodgson and Woods (1969) for the cylindrical drop model.

For all three models, our linear stability estimate for the coalescence time t_c is in better agreement with the available experimental data than is the elapsed time t_∞ between the formation of a dimpled film and its drainage to zero thickness at the rim in the absence of instabilities.

SCOPE

The rate at which drops or bubbles suspended in a liquid coalesce is important to the preparation and stability of emulsions, of foams and of dispersions, to liquid-liquid extraction, to the formation of an oil bank during the displacement of oil from a reservoir rock, and to the displacement of an unstable foam used for mobility control in a tertiary oil recovery process.

On a smaller scale, when two drops (or bubbles) are forced to approach one another in a liquid phase or when a drop is driven through a liquid phase to a fluid-fluid interface, a thin liquid film forms between the two interfaces and begins to drain. As the thickness of the draining film becomes sufficiently small (about 1,000 Å), the effects of the London-van der Waals forces and of any electrostatic double layer become significant. Depending upon the sign and the magnitude of the disjoining pressure attributable to the London-van der Waals forces and the repulsive force of any electrostatic double layer, there may be a critical thickness at which the film becomes unstable, ruptures and coalescence occurs.

Lin and Slattery (1982b) considered the early stage of this coalescence process, when the draining film is sufficiently thick that the effects of the London-van der Waals forces and of any electrostatic double layer can be neglected. To simplify the

J. Chen is presently with Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877.