To retain the advantage of sparsity, U^{-1} is generated from

$$U^{-1} = U_2^{-1} U_3^{-1} \ldots U_n^{-1} \qquad (A18)$$

where $U = U_n U_{n-1} \ldots U_2$ is a trivial factorization according to (A15). Equations (A17) and (A18) constitute the elimination form of the inverse which corresponds to the Gaussian elimination.

A further discussion of PFI and EFI may be found in the the paper by Brayton, Gustavson, and Willoughby (1970).

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Part II. A Performance Evaluation Based on the Simulation of a Natural Gas Liquefaction Process.

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SPARSCODE was evaluated based on the simulation of natural gas liquefaction using multicomponent refrigerants. Results obtained on four cases containing 179 to 573 equations show a computing time reduction by a factor of 40 to 250 in equation solving and an overall reduction by a factor of 4 to 30 for the simulation.

SCOPE

In the precursor to this paper, we outlined a strategy for solving large sparse systems of nonlinear equations. This strategy has been implemented and validated on a CDC 6400 computer. We shall refer to this computer code as SPARSCODE (sparse computation system for process design).

In this paper, we address the question of how to apply SPARSCODE to solve realistic process problems and how to evaluate its computational performance. In our experience, the importance of this type of investigation cannot be overemphasized. Real process applications are never entirely straightforward. Unlike artificial mathematical problems, we have to consider both physical and mathematical approximations of reality and balance the fidelity of the model against its impact on problem dimensionality. In a real process, the thermophysical and transport properties of the system must play a vital role in the mathematical formulation and computed results. We always have to weigh the adequacy of data representation against its computational complexity. Also, such problems as discontinuities in physical phenomena or property correlations cannot be easily anticipated in an artificial mathematical problem but may be extremely important in real life applications. It is through realistic applications that one gains a perspective of relative importance and interrelationship among the various factors which affect computational difficulties. Without such evaluations, one can easily develop esoteric computational techniques which bear little relationship to real problems.

A major difficulty in carrying out such an investigation is the availability or accessibility of suitable problems. In this case, we require the benchmark problem not only to possess the typical attributes of process problems in way of thermophysical data, phase equilibrium, and nonlinearity, but it must also be irregular in its structure so that a once-for-all structural analysis such as has been applied to conventional distillation columns is either not obvious or cannot be made at all. We also require the problem to contain irreducible systems of equations of high dimensionality. Finally, the problem must be realistic and of industrial significance. Liquefaction of natural gas (LNG) using multicomponent refrigerant (MCR) was deemed to have met all these requirements in large measures. Moreover, the simulation of LNG-MCR plants was known to present extreme convergence difficulties using conventional tearing techniques. Successful solution of this problem would therefore provide a critical test for SPARSCODE.

The specific configurations chosen for LNG-MCR were based on the process developed by Air Products and Chemicals, Inc. (Gaumer and Newton, 1971, 1972). Two basic configurations, one involving three heat exchangers and the other five heat exchangers, were used. These configurations were simulated with and without heat exchanger sectioning, making a total of four cases in the evaluation. Enthalpies and vaporization equilibrium ratios were computed using the Soave-Redlich-Kwong equation of state (Soave, 1972). To initialize the process conditions, material and enthalpy balances were first made with the assumption that the temperatures of all cooled streams leaving each heat exchanger are the same (the design problem).

By contrast, in simulating an operating process, the heat transfer areas and coefficients were specified, but the temperatures of all streams were allowed to vary freely. In these cases, the equations governing the liquefaction cycle formed an irreducible block which was solved with SPARSCODE.

The modus operandi in this investigation was as follows. First, the necessary techniques were developed for applying SPARSCODE to the benchmark problems. Second, a realistic evaluation of SPARSCODE was made through an assessment of the various factors involved in the computation.

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0001-1541-78-1608-0839-$01.25.

CONCLUSIONS AND SIGNIFICANCE

The problem dimension for the four cases studied ranged from 179 to 573 equations, with the largest irreducible block containing 551 simultaneous equations.

The symbolic phase produced very efficient inverses with less than 1% fill-ins for matrices of 1.5 to 4.5% density. Storage for numerical and structural data increased linearly with problem dimensions. Approximately 30 000 words were required for the 573 equation simulation problem. Storage for problem dependent subroutines was considerably reduced and made independent of problem dimensions by equation indexing and finite-difference approximation. For the LNG problem, the total program storage was less than 17 000 words.

The operation count for solving the linearized equations was reduced by a factor of 360 to 3 100 and the computing time by a factor of 40 to 250. With these drastic reductions, the computing time became dominated by thermophysical property evaluation. The overall computing time for the simulation was reduced by a factor of 4 to 30. In all four cases, convergence was attained in less than ten iterations.

The results obtained in this investigation confirm the potency of sparse computation strategy developed in our previous papers (Part I, and Lin and Mah, 1977) and provide a realistic and quantitative measure of the performance of SPARSCODE. With these techniques, it is now possible to tackle a large class of chemical engineering problems hitherto inaccessible to practical computation.

THE LNG-MCR PROCESS AS A BENCHMARK PROBLEM

The objective of this investigation is to evaluate the effectiveness of SPARSCODE as a computational tool for solving large process problems. Since the performance of such a computational tool is influenced to a large extent by the requirements of the applications, we must use realistic process problems as the benchmarks in such an evaluation. As an integral part of this investigation, we shall also attempt to discover the requirements of the problems insofar as they affect the performance of the computational tool and to devise techniques for coping with them.

The desired attributes of a benchmark problem are firstly those which typify a large class of process problems. It should be a continuous process involving material streams of more than one phase, it should require the computation of a reasonable range of thermophysical properties, and it should be nonlinear in its mathematical behavior. In addition, it should also be of a complexity which makes it either difficult or impossible to solve without sparse computation techniques. One such attribute is high problem dimensionality. Large systems of simultaneous nonlinear equations make enormous demands on computing time and storage. But SPARSCODE is designed specially to tackle such problems. Also, if the system of equations does not possess a regular structure, a precedence order cannot be determined a priori. Such a problem would provide a critical test of the effectiveness of the HP algorithms (Lin and Mah, 1977). Finally, it is desirable that the benchmark problem be realistic and of industrial importance.

One problem which possesses all these qualifications is the liquefaction of natural gas using multicomponent refrigerant (LNG-MCR). With reference to Figure 1, the natural gas (NG) passes through a cascade of multistream heat exchangers which are chilled by mixed refrigerants of successively lighter compositions and lower temperatures. The MCR from the compressor discharge is partially liquefied against cooling water and separated in a flash drum. The liquid (RL), primarily heavier hydrocarbons, is subcooled and then flashed down to suction pressure to provide refrigeration in the first (warmest) exchanger. After pressure reduction, it joins with the return refrigerant (RR) stream from colder exchangers to proceed to the compresssor suction. The vapor (RV) from the refrigerant flash drum is cooled, partially con-

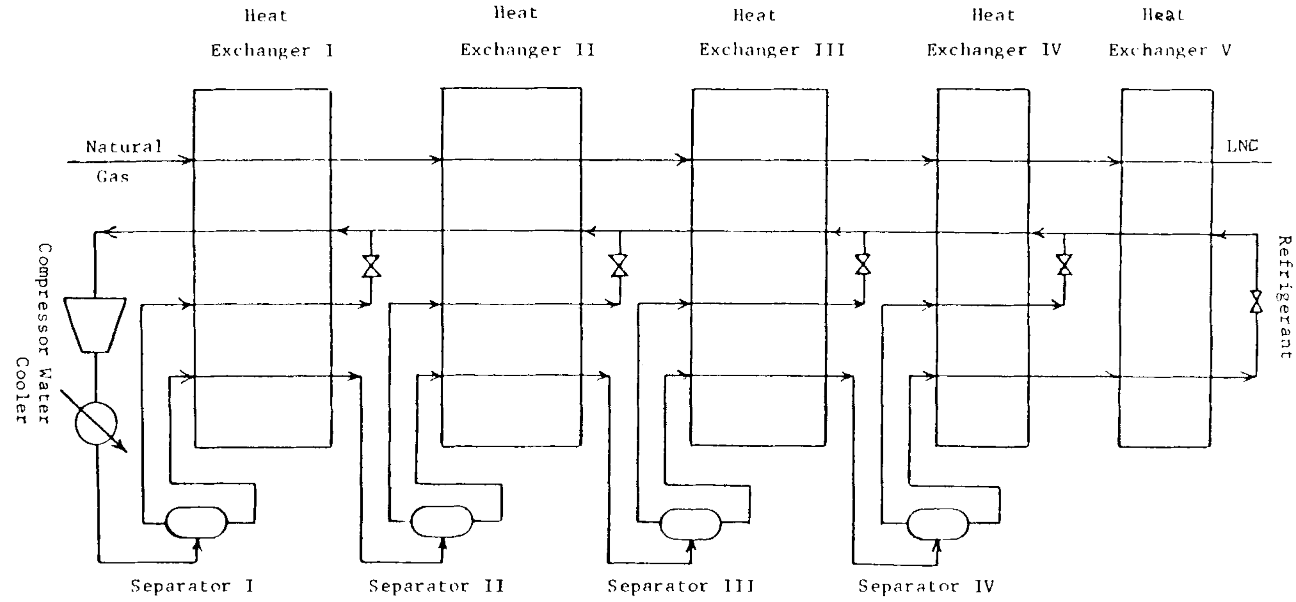


Fig. 1. Liquefaction of natural gas using multicomponent refrigerants.

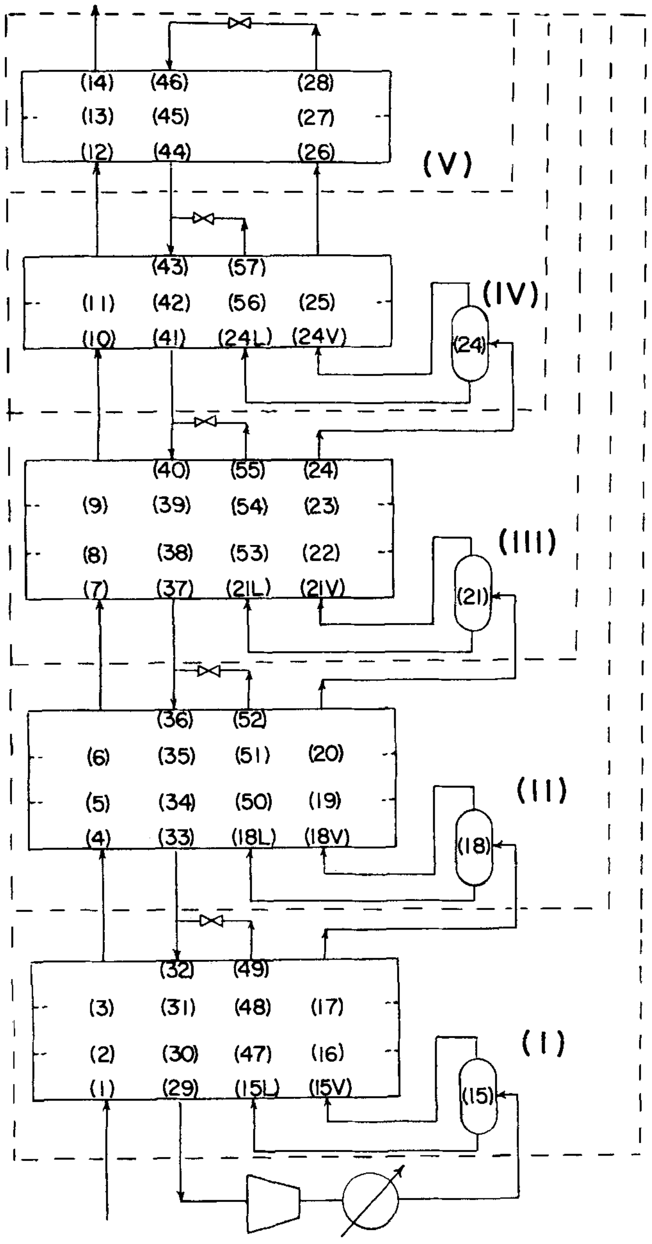


Fig. 2. Stream labels and design calculation sequence for case IV.

densed, and separated in the next flash drum, and the cycle is repeated. At the last stage, the MCR consists mainly of nitrogen and methane; no refrigerant separation is used.

LNG-MCR cycles similar to the above have been successfully applied to at least three large base load plants abroad and a number of smaller peak shaving plants in the United States and Canada (Kinard and Gaumer, 1973). The process described above is essentially a simplified version of the Air Product process (Gaumer and Newton, 1971, 1972). The advantages claimed for these processes are: lower capital investment which results from the ability to utilize fewer but larger pieces of equipment, notably compressors and heat exchangers, and self-sufficiency with regard to refrigerants which consist of components normally found in natural gas and the atmosphere. The first point is clearly important because of the large investment involved. The second point is important for base load plants which are usually situated at remote locations.

From a computational viewpoint, the modeling of LNG-MCR process offers some very challenging problems. It requires accurate thermophysical properties to predict enthalpies and phase equilibria at low temperatures (down to 110°K) and moderately high pressures ($\sim 4 \times 10^6 N/m^2$). It is highly nonlinear, not only because of the nonideal thermophysical properties but also because the refrigerant flow distribution depends strongly on the separator temperatures. Finally, for the simulation of an operating LNG-MCR plant, the equations in the MCR cycle form an irreducible system of a high dimension.

THE DESIGN PROBLEM

A typical LNG-MCR simulation entails several hundred equations and variables. Because of the high dimensionality, it is very difficult to provide initial guesses needed for its numerical solution. One technique evolved in this investigation is to use the solution of the "design problem" which is much easier to solve than the "operation problem."

In the design problem, we are given the feed rate, composition, temperature and pressure, percent recovery (natural gas liquefied), pressure drops on the natural gas side, and the cooling water temperature. If we further assume a reasonable refrigerant composition, pressure levels, and temperature levels, and temperature approaches in heat exchangers, then the remaining process conditions may be determined by utilizing the following structural decomposition and precedence ordering.

With reference to Figure 2, we note that at steady state the flow rate and overall composition of the forward flowing refrigerant leaving any exchanger, say (18), must be exactly the same as those of the return refrigerant entering the same exchanger, say (33). The two streams differ only in temperatures and fractions vaporized. Also, in the design problem we are free to assume any relationship among the temperatures of the exit hot streams. To simplify the calculations, we choose to make them equal.

With this simplification, the calculation procedure is as follows:

1. From the overall enthalpy balance (box I in dotted lines) calculate the refrigerant flow rate, the cooling water flow rate, and the compressor horsepower.
2. Determine the temperature, compositions and flow rates of the two streams (15V and 15L) leaving the first separator by equilibrium flash.
3. Assume a refrigerant temperature at (18) and calculate the return refrigerant temperature at (33) from enthalpy balance around box II.
4. Check the temperature approach. If necessary, adjust the temperature at (18) and repeat step 3.
5. Repeat steps 2 to 4 using enthalpy balances around boxes III, IV, and V.

The solution to the design problem yields a consistent set of process conditions which can then be used to initialize the operation problem.

SIMULATION TECHNIQUES

Estimation of Thermophysical Properties

The LNG-MCR simulation is dominated by phase equilibrium and enthalpy calculations. It makes severe demands not only on the accuracy of the thermophysical property estimation method but also on its computational speed and robustness. Two types of estimation methods were considered in this investigation. The first method (Zellner et al., 1970) uses the virial equation of state to represent the vapor phase and the four-suffix Margules equation to correlate the liquid phase activity coefficients.

TABLE 1. PROCESS DATA FOR LNG-MCR SIMULATION

Natural gas feed

Composition (mole %) = 2.31 N_2, 93.04 CH_4, 3.63 C_2H_6, 0.77 C_3H_8, 0.25 C_4H_{10}
Pressure (N/m^2) = 4.05×10^6
Flow rate (kg-mole/s) = 4.163

Multicomponent refrigerant

Cases I and III (three exchangers)
  Composition (mole %) = 17.46 N_2, 55.11 CH_4, 25.19 C_2H_6, 1.00 C_3H_8, 1.24 C_4H_{10}
  Flow rate (kg-mole/s) = 9.916
Cases II and IV (five exchangers)
  Composition (mole %) = 10.44 N_2, 37.26 CH_4, 31.82 C_2H_6, 3.50 C_3H_8, 16.98 C_4H_{10}
  Flow rate (kg-mole/s) = 18.14
Pressures (N/m^2) = 4.054×10^6 high, 5.516×10^5 low

Heat transfer areas (m^2)

		Case I			Case III	
Exchanger No.	NG	RV	RL	NG	RV	RL
1	2 678	1 967	9 608	3 × 1 423	3 × 766.7	3 × 3 160
2	4 705	1 087	1 724	3 × 1 258	3 × 410.0	3 × 473.8
3	5 011	1 805	—	2 × 2 400	2 × 914.9	—

		Case II			Case IV	
Exchanger No.	NG	RV	RL	NG	RV	RL
1	3 937	5 692	13 376	3 × 1 312	3 × 2 218	3 × 4 459
2	1 526	5 901	29 139	3 × 1 831	3 × 2 299	3 × 9 713
3	2 690	1 968	9 608	3 × 1 055	3 × 766.7	3 × 3 203
4	4 695	1 630	1 725	2 × 1 565	2 × 973.1	2 × 862.3
5	5 012	1 805	—	2 × 2 506	2 × 902.5	—

Heat transfer coefficients ($J/m^2 \cdot s \cdot {}^\circ K$)

Vapor to boiling liquid = 113.6
Liquid to boiling liquid = 85.2
Condensing vapor to boiling liquid = 851.8

Enthalpy change of RR stream through compressor and cooler (W)

Cases I and III = 3.796×10^7
Cases II and IV = 5.569×10^7

This method has been used in the design of low temperature heat exchangers with "temperature difference as small as 2°F" and found to give good predictions (Zellner et al., 1970). The second method uses a single equation of state, Soave-Redlich-Kwong (Soave, 1972), to represent both vapor and liquid phases. West and Erbar (1973) compared it with three other competitive equations of state (BWR-Starling-Han, Lee-Erbar-Edmister, and Robinson-Chao) and found it "to give the most reliable results of K values, enthalpy departures, and entropy departures over the broadest range of temperature and pressure conditions" for light hydrocarbon mixtures. More recently, Tarakad and Danner (1976) have found the Soave-Redlich-Kwong equation to yield reliable enthalpy estimates for mixtures including nitrogen-methane.

On the basis of accuracy of prediction, there seems to be little to choose between these two methods. However, our own computational experience showed that the Soave-Redlich-Kwong method was more than ten times faster than the Zellner-Claitor-Prausnitz method. It also appeared to be more robust near the critical region. We have therefore selected it for use in our simulation.

Modeling of Heat Exchangers

Although the natural gas enters the cryogenic exchangers as a superheated vapor, much of the heat transfer in the exchangers takes place between condensing vapors and boiling liquids of varying compositions. Moreover, the apparent temperature driving force is known to be modified by the effects of simultaneous heat and mass transfers. A rigorous procedure for computing heat transfer coefficients is clearly out of question for this investigation. Nor is it indeed necessary for an analysis of an operating plant for which the primary interest is in the relative trends rather than absolute magnitudes. However, to account for the change of process conditions, we use three different overall heat transfer coefficients, depending on whether the hot stream is a superheated vapor, a condensing vapor, or a subcooled liquid. The values of these coefficients are given in Table 1. We also divide each exchanger into several sections of equal areas for each stream. The sectioning permits a better approximation of the temperature driving force but increases the number of equations and variables. If a phase change of a hot stream occurs within a section, the overall heat transfer coefficient is taken to be the average of the heat transfer coefficients for the two prevailing sets of conditions.

Phase Changes

The symbolic rearrangement of equations and variables of LNG-MCR simulation is based on the formulation which assumes all streams to have two phases except for the liquid streams from the flash separators. However, in the course of iterations, certain temperature changes may cause some streams to change from two phases to one phase or vice versa. These changes alter the number and structure of equations. For a two-phase stream, the compositions are related by the following equations:

$$lx_i + (1-l)y_i = z_i, \quad i = 1, \ldots, m \tag{1}$$

$$y_i/x_i = K_i, \quad i = 1, \ldots, m \tag{2}$$

$$\sum_{i=1}^{m} y_i = 1 \tag{3}$$

whereas for a vapor stream and for a liquid stream, the governing equations are

$$y_i = z_i, \quad i = 1, \ldots m \tag{4}$$

$$x_i = z_i, \quad i = 1, \ldots m \tag{5}$$

respectively. Moreover, K_i is undefined for a single-phase stream. To avoid the necessity of repeating the symbolic processing, the following procedure was devised:

1. *a.* Set $y_i = z_i$, $x_i = 0$, and $l = 0$ if the temperature indicates that the stream is in vapor phase.

b. Set $x_i = z_i$, $y_i = 0$, and $l = 1$ if the temperature indicates that the stream is in liquid phase.

2. In either case, set the diagonal elements corresponding to the flash of the permuted Jacobian matrix equal to one and all other elements in the same rows and columns to zero.

3. Flash the stream to determine x_i, y_i, and l if a reverse change from one phase to two phases is indicated.

Equation Indexing

The sparse computation techniques discussed in Part I were designed to reduce storage requirements for numerical and structural data. But for large process simulation problems, the instructions for function and Jacobian evaluations can also take up enormous storage in the form of user supplied subroutines. It was estimated that for the largest problem we have studied, some 12 000 words of memory would be required for the subroutine UF (equations or function evaluations) and another 84 000 words for the subroutine UJ (partial derivative evaluations).

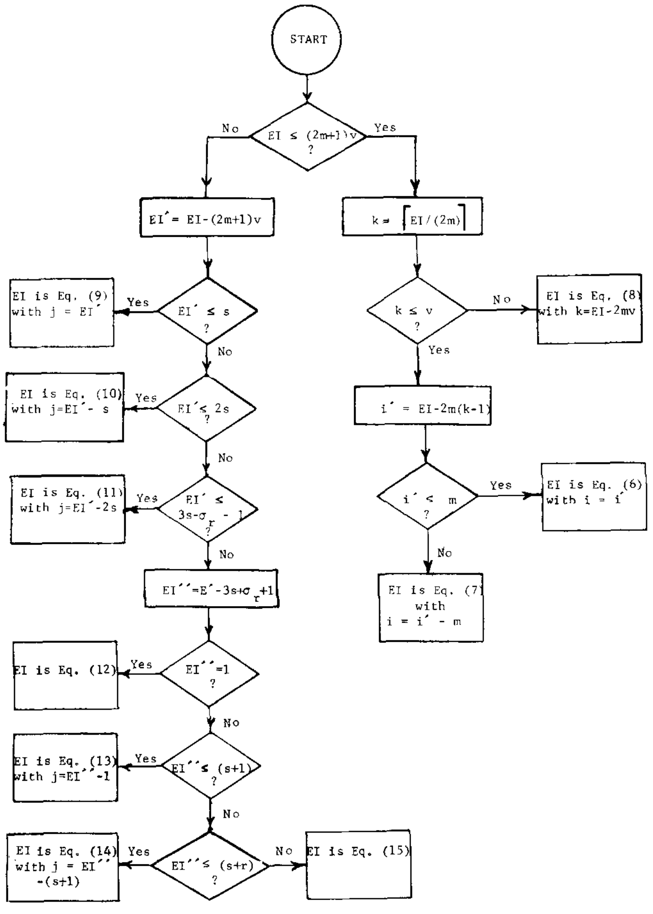


Fig. 3. Flow chart for equation indexing.

The storage required for UJ was almost completely eliminated by using numerical perturbation to generate finite-difference approximations to the partial derivatives. Finite-difference approximations are generally preferable for complex process systems for which the analytical expressions of partial derivatives are lengthy and difficult to check and debug. It is practically the only approach if parameters in the equations are defined by subroutines and procedures.

The storage required for UF was greatly reduced by equation indexing, which makes this memory requirement independent of problem dimensionality. With reference to Figure 2, the following labeling scheme was used, bearing in mind that the streams only change their conditions through pressure changes or heat exchanges and that no heat or material loss is assumed in the model:

1. The points on each of the four streams (NG, RV, RR, and RL) are numbered consecutively in the direction of decreasing temperatures.

2. The points on each stream are grouped together and the groups are labeled in the order NG, RV, RR, and RL.

3. The RL streams from the flash separators carry the same numerical labels as the corresponding RV streams but are distinguished from the latter with an additional label L instead of V, for example, 15L and 15V.

Since the RL streams will always be in liquid phase, the total number of flashes is given by $v = 3(s + 1) + (r - 1)$, where r is the number of heat exchangers and s is the number of heat exchanger sections. Similarly, the total number of independent enthalpy balances is $4s - \sigma_r + r$.

With this labeling scheme, the equations for the liquefaction cycle are arranged in the following order:
Equilibrium flash:

$$\left.\begin{aligned} l_k x_{ik} + (1-l_k)y_{ik} &= z_{ik}, \qquad (6)\\ i &= 1, \ldots, m \\ y_{ik}/x_{ik} = K_{ik}, \quad i &= 1, \ldots, m \qquad (7) \end{aligned}\right\} k = 1, \ldots, (3s + r + 2)$$

$$\sum_{i=1}^{m} y_{ik} = 1, \quad k = 1, \ldots, (3s + r + 2) \tag{8}$$

Enthalpy balance for NG streams:

$$F\Delta H_{\alpha j} = U_{\alpha j} A_{\alpha j} \Delta \overline{T}_{\alpha j}, \quad j = 1. \ldots, s \tag{9}$$

Enthalpy balance for RV streams:

$$G \prod_{k=1}^{t(j)} (1 - \lambda_k) \Delta H_{\beta j} = U_{\beta j} A_{\beta j} \Delta \overline{T}_{\beta j}, \quad j = 1, \ldots, s \tag{10}$$

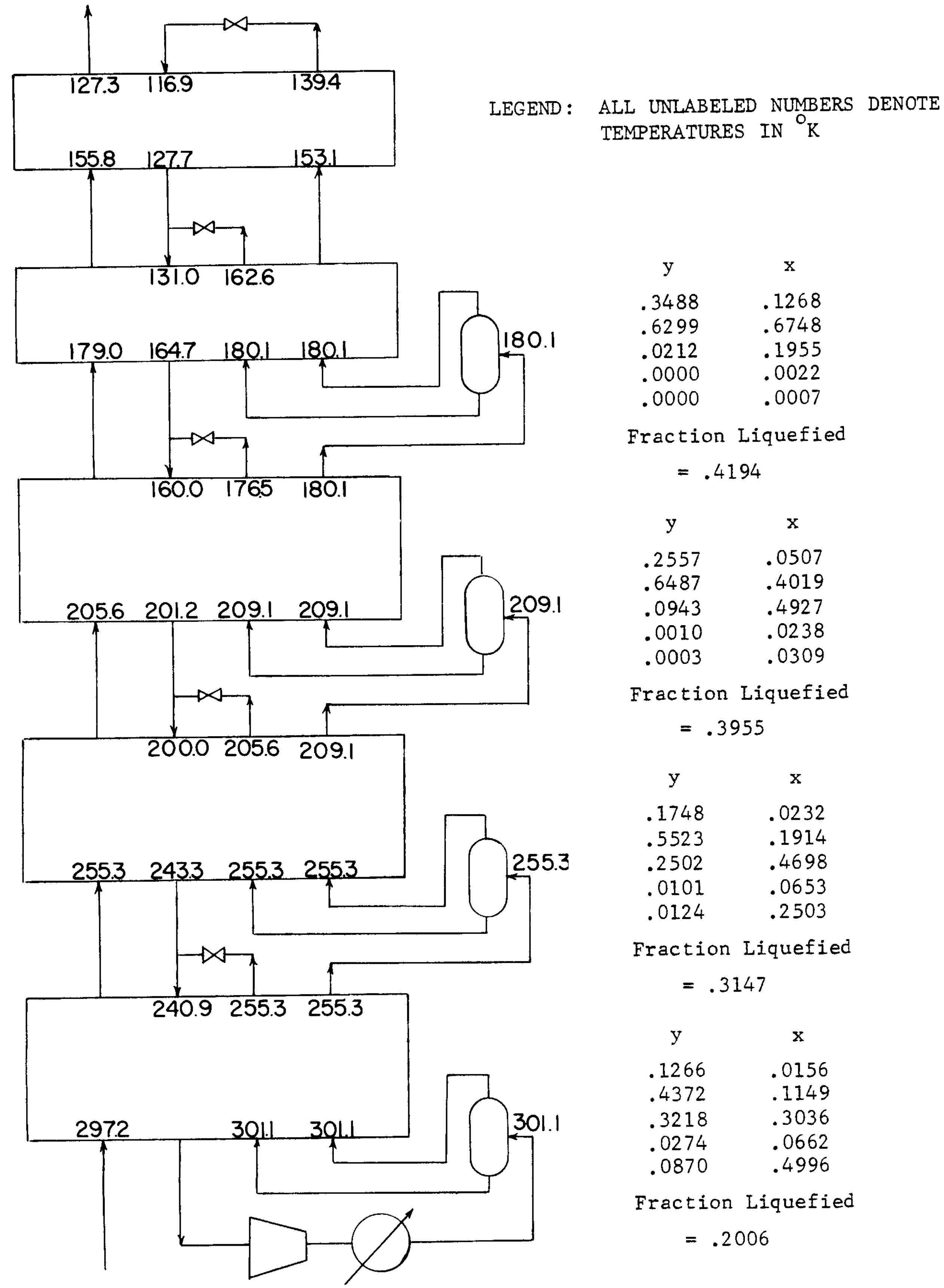
Enthalpy balance for RL streams:

$$G \prod_{k=1}^{t(j)} \lambda_k \Delta H_{\gamma j} = U_{\gamma j} A_{\gamma j} \Delta \overline{T}_{\gamma j}, \quad j = 1, \ldots, s - (1 + \sigma_r) \tag{11}$$

Enthalpy balance for RR streams:

$$G(H_{2s+3} - H_{s+2}) = Q \tag{12}$$

$$G \prod_{k=0}^{t(j)-1} (1 - \lambda_k) \Delta H_{\delta j} = U_{\alpha j} A_{\alpha j} \Delta \overline{T}_{\alpha j} + U_{\beta j} A_{\beta j} \Delta \overline{T}_{\beta j} + U_{\gamma j} A_{\gamma j} \Delta \overline{T}_{\gamma j}, \quad j = 1, \ldots, s \tag{13}$$



LEGEND: ALL UNLABELED NUMBERS DENOTE TEMPERATURES IN °K

y	x
.3488	.1268
.6299	.6748
.0212	.1955
.0000	.0022
.0000	.0007

Fraction Liquefied = .4194

y	x
.2557	.0507
.6487	.4019
.0943	.4927
.0010	.0238
.0003	.0309

Fraction Liquefied = .3955

y	x
.1748	.0232
.5523	.1914
.2502	.4698
.0101	.0653
.0124	.2503

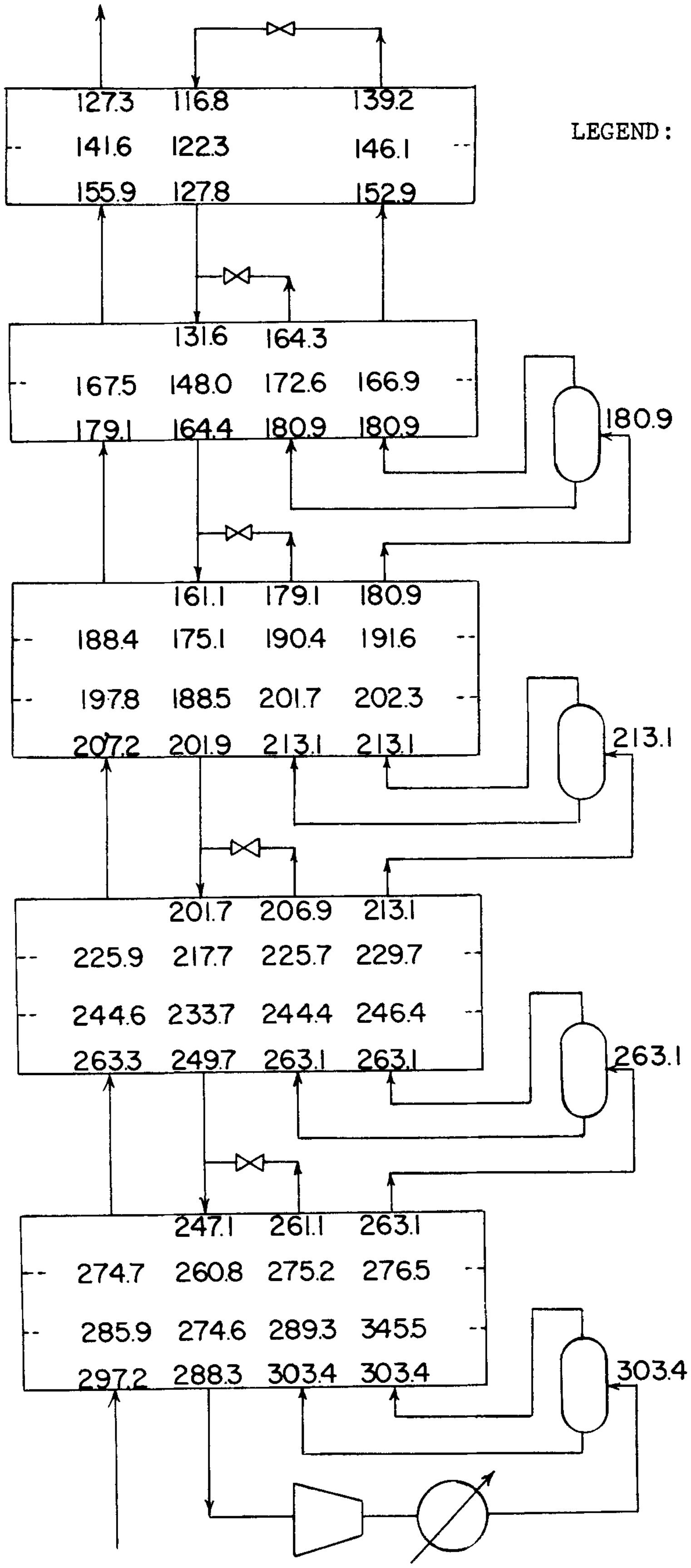
Fraction Liquefied = .3147

y	x
.1266	.0156
.4372	.1149
.3218	.3036
.0274	.0662
.0870	.4996

Fraction Liquefied = .2006

Fig. 4. Initial process conditions for case II.

$$\prod_{k=0}^{t(j)-1}(1-\lambda_k)H_{p(j)} = \prod_{k=1}^{t(j)}(1-\lambda_k)H_{p(j)+1} + \prod_{k=1}^{t(j)}\lambda_k H_{q(j)}, \quad j = 1 \ldots, (r-1) \qquad (14)$$



LEGEND: ALL UNLABELED NUMBERS DENOTE TEMPERATURES IN °K

y	x
.3490	.1224
.6281	.6610
.0229	.2126
.0001	.0029
.0000	.0011

Fraction Liquefied
= .4451

y	x
.2481	.0465
.6428	.3728
.1073	.5083
.0013	.0289
.0005	.0434

Fraction Liquefied
= .4147

y	x
.1640	.0212
.5301	.1725
.2747	.4487
.0129	.0681
.0184	.2895

Fraction Liquefied
= .2895

y	x
.1243	.0154
.4308	.1125
.3230	.2967
.0282	.0654
.0937	.5100

Fraction Liquefied
= .1829

Fig. 5. Initial process conditions for case IV.

$$H_{3s+r+2} = H_{2s+2} \qquad (15)$$

An additional eleven equations are included in the program to specify feed temperature, feed composition, and

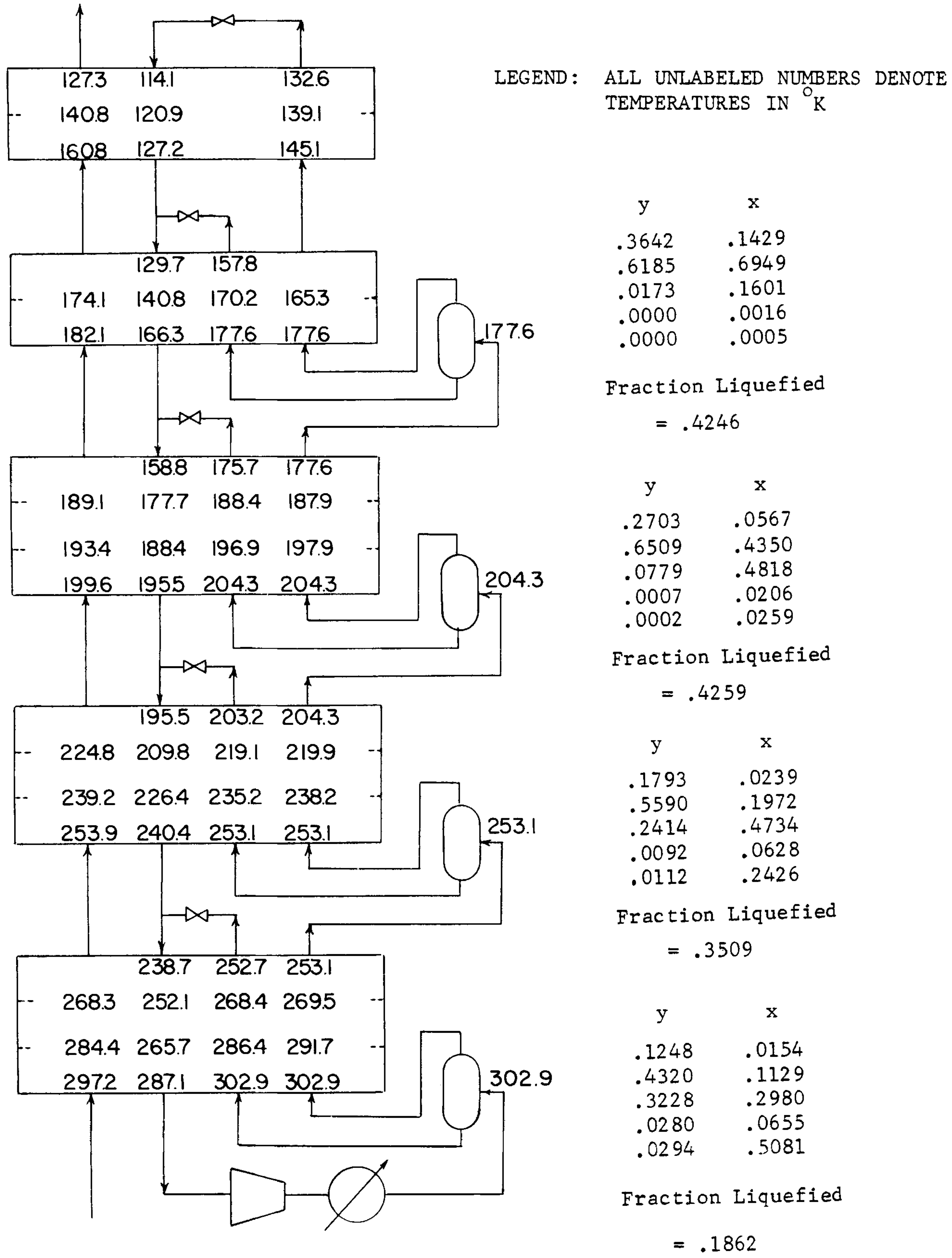


Fig. 6. Converged process conditions for case IV.

refrigerant composition. In the input to SPARSCODE, the variables are arranged in the following orders: first, in the order of flashes, the vapor mole fractions $y_{ik}(i = 1, \ldots, m)$, the liquid mole fractions $x_{ik}(i = 1, \ldots, m)$ for each of the $3s + r + 2$ flashes, then the corresponding fractions liquefied $l_k(k = 1, \ldots, 3s + r + 2)$, and finally the temperatures, feed, and refrigerant compositions.

For the example shown in Figure 2, $m = 5$, $r = 5$, $\sigma_1 = \sigma_2 = \sigma_3 = 2$, $\sigma_4 = \sigma_5 = 1$, $s = 13$, $\lambda_1 = l_{15}$, $\lambda_2 = l_{18}$, $t(4) = 2$, $t(10) = 4$, $p(2) = 36$, $q(2) = 52$. By

TABLE 2. SYMBOLIC PHASE RESULTS ON SPARSE MATRICES ASSOCIATED WITH LNG-MCR PROBLEMS

Problem	I	II	III	IV
Number of equations	179	278	364	573
Number of nonzero elements	1 449	2 382	3 152	5 079
Number of fill-ins	277	591	644	1 150
Density of matrix, %	4.52	3.08	2.38	1.55
Densityl of EFI, %	5.39	3.85	2.86	1.90
Operation counts (solution of linearized equations)	5 467	9 792	12 303	20 451
Ratio of full matrix operations, %	0.281	0.135	0.0759	0.0324

using the flow chart shown in Figure 3, we can identify each equation by one equation index (EI). For example, if the equation index is 238, then it is Equation (7) with $i = 3$ and $k = 24$, and if the equation index is 515, then it is Equation (9) with $j = 9$, and so on. With equation indexing, the instructions for Equations (6) to (15) need be coded and stored only once in the user supplied subroutine UF, and the storage required is reduced to 1 871 words.

DISCUSSION OF RESULTS

The process data used in the LNG-MCR simulation are given in Table 1. For the operation problem, the specified variables are the flow rate and inlet conditions of the natural gas; the flow rate, pressure levels, and enthalpy changes of the refrigerant; and the heat transfer coefficients and areas. Four cases were simulated. Cases I and II involve three and five unsectioned heat exchangers, respectively, while cases III and IV consist of the same configurations with heat exchanger sectioning. The solutions to the design problems with some modifications were used to initialize cases I and II, which were, in turn, used to initialize cases III and IV, with interpolations to provide intermediate temperatures. The initial and converged process conditions for cases II and IV were shown in Figures 4 to 6. The iterations were terminated if either the Euclidean norm of the residuals was less than 10^{-6} or the numerical value of the ratio of the change of a variable to its present value was less than 10^{-8} for every variable. Convergence was attained after six, eight, six, and nine iterations for the four cases, respectively.

The performance data are summarized in Tables 2 and 3. We shall now analyze this information in terms of storage and computing time requirements. As noted in the previous section, the storage required for user supplied subroutines UF and UJ were reduced from an estimated total of 96 000 words to about 2 000 words through the use of equation indexing and finite-difference approximation of partial derivatives. An equally drastic reduction in data storage was attained with SPARSCODE. Table 2 gives the key results of the symbolic phase. The original density of the Jacobian matrix ranged from 4.52 to 1.55%. Significantly, the corresponding EFI densities were only 5.39 to 1.90%. In other words, the density increase due to fill-ins was held to less than 1% absolute or 25% of the original matrix density. This is a considerable improvement over the results obtained by Brayton et al. (1970) who reported as much as sevenfold increase in density for EFI due to fill-ins for a 300 × 300 matrix of 1% original density. The comparison clearly indicates that the HP algorithm functioned very effectively.

Table 3 gives the actual program and data storage for the four cases. Bearing in mind that the program is in overlay with the symbolic and numerical phases in two different branches, the overall program length is determined by the longer of the two branches. The results show that the program storage for the two branches and for the root segment (main program and system subroutines) are approximately equal and independent of problem dimensions. On the other hand, the data storage in both phases grows approximately linearly with problem dimensions and represents from 10 to 30% of the storage for a full matrix of corresponding dimension. It should be noted that much more than the Jacobian matrix

TABLE 3. STORAGE AND COMPUTING TIME REQUIREMENT FOR SOLVING THE LNG-MCR PROBLEMS

	Problem	I	II	III	IV
	Number of equations	179	278	364	573
Storage, words	Main program and system subroutines	7 845	7 845	7 845	7 845
	Branch 1: symbolic phase				
	Program	8 771	8 771	8 771	8 771
	Data	8 663	12 823	19 351	29 015
	Branch 2: numerical phase				
	Program	8 043	8 043	8 043	8 043
	Data	9 903	15 087	19 119	30 551
Computing time, CP s	Symbolic phase CP s (algorithm)	16.68 (HP-00)	3.66 (HP-20)	17.78 (HP-10)	10.91 (HP-20)
	Numerical phase				
	CP s/iteration:				
	Function evaluation	1.53	1.92	2.39	5.15
	Jacobian evaluation	1.48	3.16	3.69	6.37
	Solution of linearized equations	0.285	0.621	0.747	1.44

is involved in actual data storage. The full matrix storage is cited merely to provide a framework of reference.

The symbolic phase results in Table 2 also give the operation counts (floating point multiplications) for the solution of linearized equations. As a comparison, these counts are expressed as percentages of their counterparts for a full matrix for which the counts are given by $(n^3 + 3n^2 - n)/3$. Reduction by a factor of 360 to 3 100 is indicated by these values. The actual computing time for solving linearized equations is given in Table 3 in terms of CP (central processor) seconds for the CDC 6400 computer. If we take the computing time for a floating point multiplication to be 5.7×10^{-6} CP s, it can easily be shown that the computing time for solving the linearized equations is reduced by a factor of 40 to 250. If we take these two sets of results together, the implication is that there is an overhead factor of roughly ten in computing time associated with sparse computation. If we take into consideration the computing time required for function and partial derivative evaluation, the overall computing time is reduced by a factor of 4 to 30 for the four cases studied.

CLOSING REMARKS

In the specific strategy used in SPARSCODE, the computation is divided into symbolic and numerical phases, and the equations are allowed to contain parameters which may be defined by user supplied subroutines. It should be pointed out that this is not the only strategy open to sparse computation. Although the merits of these system features over the alternatives are not immediately evident, the choice turns out to be very fortunate in retrospect. The two-pass strategy has made it easy to allow for changes of equations caused by phase changes, and the provision for parameters has eliminated the necessity of including every equation in the symbolic rearrangement. Both features contribute toward greater flexibility.

As stated at the beginning, the objective of this study is to obtain a realistic assessment of the utility of SPARSCODE. Since the thrust is not to obtain any specific process result or draw any specific process conclusion, we have omitted certain aspects of process computation, such as estimation of heat transfer coefficients or checking for temperature crossovers, which are clearly of great importance in cryogenic exchanger design and simulation but whose omission would not significantly alter the fundamental characteristics of LNG-MCR simulation as a benchmark problem.

The approach advocated in this paper was first demonstrated for a specific class of problems, namely, steady state pipeline network flows (Mah, 1974). In the present investigation, the algorithms and techniques are generalized to other process applications. The dramatic reduction in computing time and storage and the relatively rapid rate of convergence provide further confirmation of the potency of sparse computation in solving process problems described by large sets of nonlinear simultaneous equations.

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NOTATION

$A_{\alpha j}, A_{\beta j}, A_{\gamma j}$ = heat transfer areas for NG, RV, and RL streams in the j^{th} section, m^2
F = natural gas flow rate, kg-mole/s
G = refrigerant flow rate, kg-mole/s
H_k = the molal enthalpy of the stream at point k in Figure 2, J/kg-mole
$\Delta H_{\alpha j}, \Delta H_{\beta j}, \Delta H_{\gamma j}, \Delta H_{\delta j}$ = enthalpy changes for NG, RV, RL, and RR streams in the j^{th} section, J/kg-mole
K_i = vaporization equilibrium ratio for component i
l = fraction liquefied
m = number of components
n = dimension of an irreducible system of equations or the dimension of a matrix
$p(j)$ = index number of the RR stream entering the j^{th} heat exchanger
Q = specified enthalpy change, W
$q(j)$ = index number of the RL stream leaving the j^{th} heat exchanger
r = number of heat exchangers
s = total number of heat exchanger sections
$t(j)$ = index number of the heat exchanger which contains the j^{th} section
$\Delta\overline{T}_{\alpha j}, \Delta\overline{T}_{\beta j}, \Delta\overline{T}_{\gamma j}$ = average temperature differences between NG, RV, RL streams and RR stream in the j^{th} section, °K
$U_{\alpha j}, U_{\beta j}, U_{\gamma j}$ = overall heat transfer coefficients for NG, RV, and RL streams in the j^{th} section, J/m^2·s·°K
v = $3s + r + 2$, the total number of flashes
x_i = mole fraction of component i in the liquid
y_i = mole fraction of component i in the vapor
z_i = mole fraction of component i in the combined phases
λ_k = fraction liquefied in the k^{th} separator, $\lambda_o = 0$ and $\lambda_n = 0$
σ_j = number of sectioning in the j^{th} heat exchanger
$\lceil x \rceil$ = smallest integer greater than or equal to x

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