A Simultaneous-Modular Approach to Process Flowsheeting and Optimization

Part II: Performance on Simulation Problems

The performance of the simultaneous-modular approach on five simulation problems, ranging in complexity from very simple to moderately complex, is studied. Numerical experiments comparing different computational strategies for implementing the simultaneous-modular approach are also performed. Full-block perturbation is found to be the most suitable technique for obtaining the flowsheet-level Jacobian. On process simulation problems the simultaneous-modular approach, as implemented in SIMMOD, is found to be as reliable as the sequential-modular approach, and competitive with or sometimes much better than the sequential-modular approach in terms of computational efficiency.

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SCOPE

This is the second in a series of papers in which we present a comprehensive study and critical evaluation of the simultaneous-modular approach for process flowsheeting and optimization problems. In Part I, we discussed the theory underlying several possible means of implementing the simultaneous-modular approach, and described our own implementation SIMMOD.

In this paper we use SIMMOD to evaluate the performance of the simultaneous-modular approach and the computational strategies for implementing it on process simulation problems. More specifically, we address the following questions:

1. In the sequential-modular approach, direct or accelerated substitution is used to converge the flowsheet-level problem. Since in the simultaneous-modular approach, linearization methods are used to solve the nonlinear equations, the simultaneous-modular approach will probably require fewer iterations to converge the same problem than the sequential modular approach. However because the evaluation of a flowsheet-level Jacobian is needed in the simultaneous-modular approach, it is not clear whether it can compete with the sequential-modular approach in terms of overall efficiency.

2. Direct and acclerated substitution are generally quite reliable solution methods, though even accelerated substitution is typically rather slow to converge. Since the flowsheet-level equation solving methods used in the simultaneous-modular approach typically require a reasonably good initial guess, it is not clear whether the simultaneous-modular approach will be as reliable as the sequential-modular approach.

3. The diagonal-block perturbation technique of Mahalec et al. (1979) for evaluating an approximate Jacobian for the flowsheet-level requires only a moderate amount of computation compared to the full-block perturbation and direct different approximation techniques. However if the approximation from the diagonal-block perturbation technique is not good enough, more iterations may be needed, or in the worst case, the nonlinear equation solver may fail. It is not clear whether this approach is better than full-block perturbation or direct difference approximation.

4. The use of approximate physical property models for derivative evaluations and rigorous models for function evaluations has frequently been suggested. If this strategy is adopted for approximating the flowsheet-level Jacobian, will it significantly affect the efficiency and reliability of the simultaneous-modular approach?

5. The selection of the tear set sometimes has a strong effect on the convergence of the sequential-modular approach. Does it have a similar effect on the simultaneous-modular approach?

6. Does the inclusion of design specifications in the flowsheet-level problem significantly increase the number of iterations required by the simultaneous-modular approach?

Five benchmark problems are used in this study. These problems are taken from the literature so that comparisons with other approaches can be made. Problem 1 is the well-known four-flash-unit system studied by Cavett (1963). Problems 2, 3 and 4 are examples 2, 3, and 4 in the CHESS User's Guide (Motard and Lee, 1971). Problem 2 is a cyclopentadiene recovery process. Problem 3 is a simple ethylene process. Problem 4 is the raw product recovery section of a natural gasoline

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plant. Problem 5 is a light hydrocarbons recovery process. This is exercise 25 in the FLOWTRAN exercise book (Clark, 1977). Of the five problems studied, Problem 3 is a very easy problem for the sequential-modular approach, Problem 2 is slightly harder, while the remaining three problems are fairly difficult.

CONCLUSIONS AND SIGNIFICANCE

Results of studies on five benchmark problems show that, as implemented in SIMMOD, the simultaneous-modular approach is not only as reliable as the sequential-modular approach, but is computationally as efficient if not more so, especially on the more complex problems. Only on one very simple problem (Problem 3) does the sequential-modular approach seem to be advantageous.

Numerical experiments using SIMMOD indicate that: 1. Of the three options considered for calculating the Jacobian, full-block perturbation is the best, diagonal-block perturbation being too unreliable, and direct difference approximation too expensive. 2. The use of simple physical property models in calculating the Jacobian is effective in reducing the computation time and seems to have no effect on reliability. 3. The choice of tear set has little effect on the performance of the simultaneous-modular approach. 4. For controlled simulations the simultaneous-modular approach is particularly attractive, and it offers potential savings on parametric simulation studies as well.

INTRODUCTORY REMARKS

Throughout this study the following options are used in SIMMOD unless specified otherwise:

1. All thermodynamic properties are calculated using the Peng-Robinson (1976) equation of state with all binary parameters set equal to zero.
2. Irreducible blocks and tear sets are found automatically by the method described in Part I.
3. Before performing simultaneous-modular iterations on

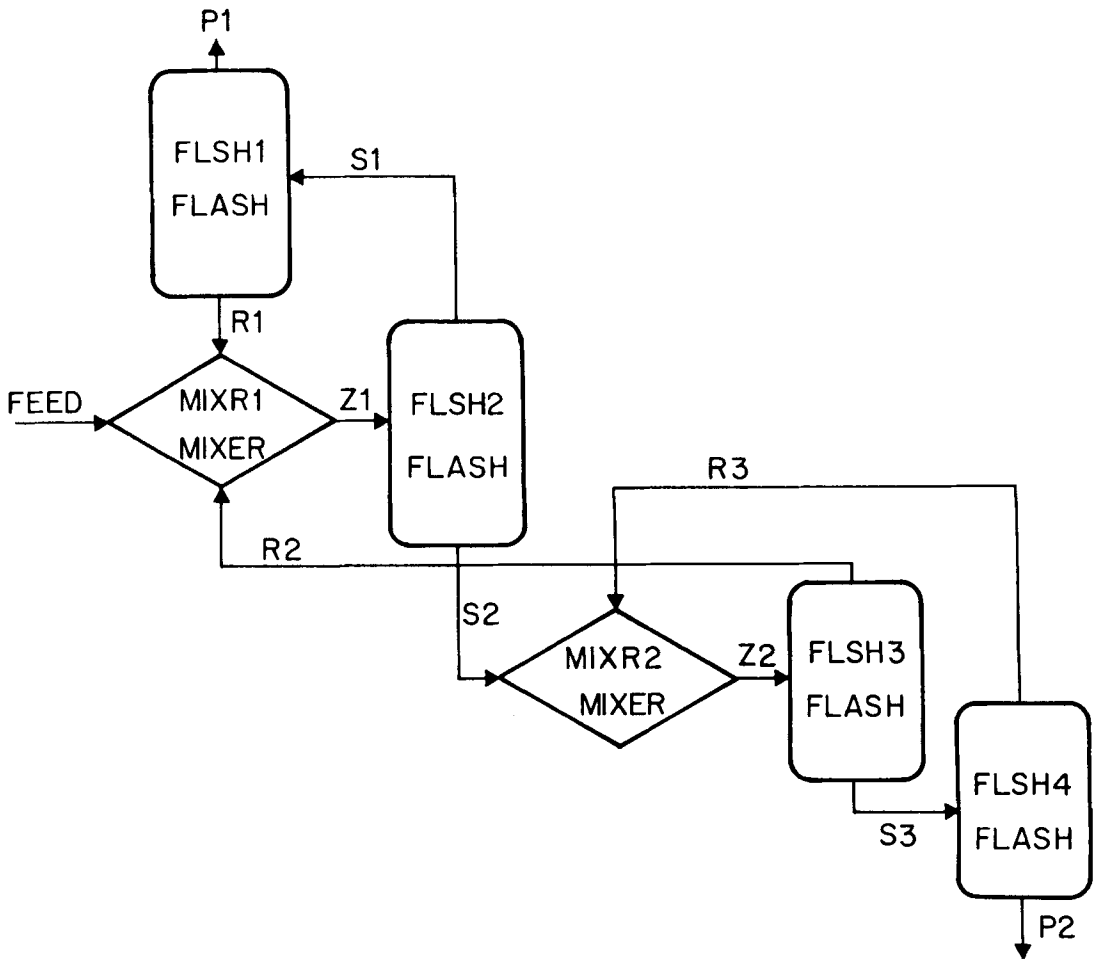

Figure 1. Block diagram for Cavett's four flash unit process (Problem 1). In each block the user-assigned name appears first, followed by the SIMMOD module name. User-assigned stream names are also shown.

TABLE 1. PROBLEM SPECIFICATIONS FOR CAVETT PROBLEM

Stream FEED:	Temperature	322 K
	Pressure	0.439 MPa
	Component flow rates:	
	N_2	0.04523 kgmol/s
	CO	0.62697 kgmol/s
	H_2S	0.04285 kgmol/s
	Methane	0.37822 kgmol/s
	Ethane	0.30246 kgmol/s
	Propane	0.28927 kgmol/s
	i-Butane	0.07628 kgmol/s
	n-Butane	0.19443 kgmol/s
	i-Pentane	0.09980 kgmol/s
	n-Pentane	0.14266 kgmol/s
	n-Hexane	0.22282 kgmol/s
	n-Heptane	0.32913 kgmol/s
	n-Octane	0.23289 kgmol/s
	n-Nonane	0.21073 kgmol/s
	n-Decane	0.10501 kgmol/s
	n-Undecane	0.15335 kgmol/s
MIXR1	Mixer	
FLSH1	Isothermal flash unit	
	Flash temperature = 311 K	
	Flash pressure = 5.62 MPa	
FLSH2	Isothermal flash unit	
	Flash temperature = 322 K	
	Flash pressure = 1.96 MPa	
MIXR2	Mixer	
FLSH3	Isothermal flash unit	
	Flash temperature = 309 K	
	Flash pressure = 0.493 MPa	
FLSH4	Isothermal flash unit	
	Flash temperature = 303 K	
	Flash pressure = 0.191 MPa	

each irreducible block, we set all tear stream variables equal to zero, ignore free variables and design specifications, and perform three sequential-modular iterations.

4. The relative convergence test $\|\Delta x\| \leq \delta \max[\|x\|, 1.0]$ is used, where x is the vector of variables being iterated on and $\|\bullet\|$ indicates the Euclidian norm. The relative convergence tolerance δ is 10^{-6} in the module calculations and 10^{-4} in the flowsheet-level calculations. The perturbation factor in the Jacobian evaluation is 10^{-3}.

5. All runs using SIMMOD were done on a CDC Cyber 175.

It should also be noted that, unless specified otherwise, results quoted below for sequential-modular simulators are for the case in which a bounded Wegstein convergence block is used to perform the accelerated substitution iterations. Bounded Wegstein is very widely used in sequential-modular simulators and is regarded as rapidly convergent (Aspen Technology, 1982). Thus the results quoted are representative of efficient sequential-modular simulators.

PROBLEM 1: CAVETT'S FOUR-FLASH-UNIT PROBLEM

This is a test problem used by Cavett (1963). The block diagram of this problem is shown in Figure 1, and the specifications for this problem are given in Table 1. This problem has been repeatedly used to study various methods for accelerated substitution and to study the effect of different tear sets on convergence (Crowe and Nishio, 1975; Genna and Motard, 1975; Mahalec et al., 1979; Rosen and Paul, 1977; Upadhye and Grens, 1975). Twenty iterations, plus or minus a few, is generally regarded as a good performance for a sequential modular simulator on this problem.

A sample input file for SIMMOD for this problem is shown in Table 2. Basically it tells the simulator the components to use, the library subroutine to use for each unit, the input streams to each unit, the output streams from each unit, the equipment parameters for each unit, the feed stream data, the desired accuracy of the solution, the output frequency, and any other options to be used. SIMMOD will take this input file, determine a tear set if it is not provided or if only a partial tear set is given, and perform recycle calculations on each irreducible block.

For this problem SIMMOD identifies streams Z1 and R3 as tears. This tear set belongs to the same irredundant family (Upadhye and Grens, 1975) as the tear set {R1, R2, R3}, which has been studied extensively. The performance of the simultaneous-modular approach using this tear set and three different options for Jacobian evaluation is shown as runs 1–3 in Table 3. Several comments are in order:

1. The Jacobian evaluation options used (and the corresponding notations in Table 3) are direct difference approximation (Direct), full-block perturbation (Full), and diagonal-block perturbation (Diag.). These techniques have been discussed in detail previously (Chen and Stadtherr, 1985a).

2. The number of components in this problem is 16, so each stream represents 18 variables and each stream connection equation represents 18 equations. Since there are two tear streams and no free variables on runs 1–3, there are 36 equations on the flowsheet level.

3. The initialization time is the time required to perform three sequential-modular iterations. This is not necessarily a good measure of the average time per sequential-modular iteration, however, as will be seen in Problem 4.

4. The number of function evaluations performed, excluding those used for Jacobian evaluation, is $NI_{SIM} + 1$, where NI_{SIM} is the number of simultaneous-modular iterations. Each function evaluation requires one sequential modular iteration. Thus the function evaluation time is the time for $NI_{SIM} + 1$ sequential-modular iterations. The average time for doing one sequential-modular iteration is about 0.058 s for this problem. This is a better measure of the average time per sequential-modular iteration than the initialization time.

5. Using the average time per sequential-modular iteration found from the function evaluation time, one can express the Jacobian evaluation time and the overhead time for the nonlinear equation solver NEQLU (Chen and Stadtherr, 1981) in terms of an equivalent number of sequential-modular iterations. Thus for run 1, the total equivalent number of sequential-modular iterations is $3 + 4 + 1 + (2.006 + 0.136)/0.058 = 45$.

6. The nonlinear equation solver NEQLU requires a Jacobian evaluation initially but thereafter only when necessary to maintain a good rate of convergence. In most iterations NEQLU simply updates the Jacobian using Broyden's method. For runs 1 and 2, only one Jacobian evaluation was required. The number of sequential-modular iterations required to evaluate a Jacobian by direct difference approximation in SIMMOD is equal to the total number of tear variables and free variables plus one. Thus for run 1, each perturbation requires about $(2.006-0.058)/36 = 0.054$ second, so the ratio of the perturbation time to sequential-modular iteration time is about 0.93. This relatively high ratio means that because using the direct difference approximation all the calculations of a given module are not performed consecutively, as in the case of block perturbation, the calculation could not take advantage of the fact that the values of input variables to each module during Jacobian evaluation are only slightly different from the previous values. Because of this, the equivalent number of sequential iterations for run 1 is rather high, although only four simultaneous iterations are required to converge the problem.

7. The number of module calculations required to calculate a Jacobian by full-block perturbation in SIMMOD is proportional

TABLE 2. SAMPLE INPUT FILE FOR CAVETT PROBLEM—SIMULATION CASE

```
C
C  THIS IS A SAMPLE INPUT FILE FOR CAVETT PROBLEM
C
TITLE "CAVETT PROBLEM—FLASH MIXER UNITS"
RUN-OPTIONS:  SAVE-RESULTS, EXECUTION, JAC-OPT = FULL;
COMPONENTS:  N2,CO2,H2S,CH4,C2H6,C3H8,I-C4H10,N-C4H10,
             I-C5H12,N-C5H12,N-C6H14,N-C7H16,N-C8H18,
             N-C9H2O,N-C10H22,N-C11H24
PROPERTY:  PENG-ROBINSON
C
C  THIS IS THE MODULE DESCRIPTION SECTION
C
MODEL AD1 BY MIXER:  IN = FEED, R1, R2; OUT = Z1;
MODEL FLSH1 BY FLASH:  IN = S1; OUT = P1,R1:
  PARA = 1.0, 0.0, 311.0, 0.0, 5.62;
MODEL FLSH2 BY FLASH:  IN = Z1; OUT = S1,S2;
  PARA = 1.0, 0.0, 322.0, 0.0, 1.96;
MODEL AD2 BY MIXER:  IN = S2,R3; OUT = Z2;
MODEL FLSH3 BY FLASH:  IN = Z2; OUT = R2,S3;
  PARA = 1.0, 0.0, 309.0, 0.0, 0.439;
MODEL FLSH4 BY FLASH:  IN = S3; OUT = R3,P2;
  PARA = 1.0, 0.0, 303.0, 0.0, 0.191;
C
C    THIS IS THE STREAM DESCRIPTION SECTION
C
STREAM FEED:  TYPE = INPUT, T = 322, P = 0.439;
  CFLOW = 0.04523,0.62697,0.04285,0.37822,0.30246,0.28927,
    0.07628,0.19443,0.0998,0.14266,0.22282,0.32913,
    0.23289,0.21073,0.10501,0.15335;
STREAM P1:  TYPE = OUTPUT;
STREAM P2:  TYPE = OUTPUT;
C
C    OTHER INFORMATION
C
CONV-CONTROL:  DERROR = 1.0E-4, SEQUENTIAL = 3, SIMULTANEOUS = 30;
PRINT-CONTROL:  FREQUENCY = 10
END
```

to the number of unknown input variables and free variables to each module plus one. For this problem, each flash unit has one unknown input stream, so each flash calculation was performed 18 + 1 times. For run 2, the ratio of the perturbation time to the sequential iteration time is $(0.819 - 0.058)/(18 \times 0.058) = 0.73$, which is somewhat less than in the direct difference approximation case because for block perturbation all the perturbation calculations for a given module can be performed consecutively, and thus some intermediate results can be retained and reused. The equivalent number of sequential iterations for run 2 is 3 + 4 + 1 + (0.819 + 0.136)/0.058 = 25, which is quite competitive with the sequential-modular approach.

8. Two Jacobian evaluations were required by NEQLU in the diagonal-block perturbation case. The CPU time spent on Jacobian calculation was still very short. However, the program did not converge in 30 iterations because the Jacobian was not sufficiently accurate.

To study the performance of the simultaneous-modular approach on controlled simulation problems, we specified heat loads to the flash units and selected flash temperatures as free variables to meet these specifications. The input file for this controlled simulation case is shown in Table 4. Note that it is essentially the same as that for the simulation case except that specifications are specified through SPEC statements and flash temperatures are freed by FREE statements. The specified heat loads are those in the solution of the simulation problem above, while the initial values for the flash temperatures are 10 K lower than the previously specified values. The result for this controlled simulation run is shown as run 4 in Table 3. As can be seen, including the four design specifications on the flowsheet level only increases the number of iterations from four to six and increases the CPU time by only 30%. As a comparison, we introduced a control loop around each isothermal flash unit, i.e., every time a flash module is executed, it will repeatly adjust the flash temperature and perform an isothermal flash calculation until

TABLE 3. PERFORMANCE OF SIMMOD ON CAVETT PROBLEM

	Run Number				
	1	2	3	4	5
Tear Set Used	Z1,R3	Z1,R3	Z1,R3	Z1,R3	Z1,R3
Jacobian Option Used	Direct	Full	Diag.	Full	Full
Initialization Time, s	0.122	0.119	0.119	0.126	0.593
Simultaneous Iterations	4	4	30*	6	4
Function Eval. Time, s	0.286	0.287	1.807	0.418	1.088
Jacobian Eval. Time, s	2.006	0.819	0.267	1.050	3.843
NEQLU Time, s	0.136	0.143	—	0.214	0.136
No. of Eqs.	36	36	36	40	36
Equiv. No. of Sequential Iter.	45	25	—	30	26

* Did not converge.

TABLE 4. SAMPLE INPUT FILE FOR CAVETT PROBLEM—CONTROLLED SIMULATION CASE

```
TITLE "CAVETT PROBLEM—FLASH MIXER UNITS"
RUN-OPTIONS:  SAVE-RESULTS, EXECUTION, JAC-OPT = FULL;
COMPONENTS:   N2,CO2,H2S,CH4,C2H6,C3H8,I-C4H10,N-C4H10,
              I-C5H12,N-C5H12,N-C6H14,N-C7H16,N-C8H18,
              N-C9H20,N-C10H22,N-C11H24
PROPERTY:  PENG-ROBINSON
C
C     THIS IS THE MODULE DESCRIPTION SECTION
C
C
C  CHOOSE FLASH TEMPERATURE (PARAMETER 3) AS FREE VARIABLE
C  SPECIFY THE HEAT LOAD (PARAMETER 6)
C
MODEL AD1 BY MIXER: IN = FEED, R1,R2; OUT = Z1;
MODEL FLSH1 BY FLASH:  IN = S1; OUT = P1,R1;
  PARA = 1.0, 0.0, 301.0, 0.0, 5.62;
  FREE = 3 (20.0, 291.0, 331.0)
  SPEC = 6 (= −9.30557)
MODEL FLSH2 BY FLASH:  IN = Z1; OUT = S1,S2;
  PARA = 1.0, 0.0, 312.0, 0.0, 1.96;
  FREE = 3 (20.0, 302.0, 342.0);
  SPEC = 6 (= −15.6544);
MODEL AD2 BY MIXER:  IN = S2,R3; OUT = Z2;
MODEL FLSH3 BY FLASH:  IN = Z2; OUT = R2,S3;
  PARA = 1.0, 0.0, 299.0, 0.0, 0.439;
  FREE = 3 (20.0, 289.0, 329.0)
  SPEC = 6 (6.12246);
MODEL FLSH4 BY FLASH:  IN = S3; OUT = R3,P2;
  PARA = 1.0, 0.0, 293.0, 0.0, 0.191;
  SPEC = 6 (= 1.88982)
  FREE = 3 (20.0, 283.0, 323.0);
C
C     THIS IS THE STREAM DESCRIPTION SECTION
C
STREAM FEED:  TYPE = INPUT, T = 322, P = 0.439;
  CFLOW = 0.04523,0.62697,0.04285,0.37822,0.30246,0.28927,
    0.07628,0.19443,0.0998,0.14266,0.22282,0.32913,
    0.23289,0.21073,0.10501,0.15335;
STREAM P1:  TYPE = OUTPUT;
STREAM P2:  TYPE = OUTPUT;
C
C     OTHER INFORMATION
C
CONV-CONTROL:  DERROR = 1.0E-4, SEQUENTIAL = 3, SIMULTANEOUS = 30;
PRINT-CONTROL:  FREQUENCY = 10
END
```

TABLE 5. PERFORMANCE OF SIMMOD ON CAVETT PROBLEM WITH DIFFERENT TEAR SETS

	Run Number					
	1	2	6	7	8	9
Tear Set Used	Z1,R3	Z1,R3	Z1,Z2	Z1,Z2	R1,R2,R3	R1,R2,R3
Jacobian Eval. Option Used	Direct	Full	Direct	Full	Direct	Full
Initialization Time, s	0.122	0.119	0.102	0.100	0.180	0.170
Simultaneous Iterations	4	4	5	5	4	4
Function Eval. Time, s	0.268	0.287	0.347	0.347	0.291	0.299
Jacobian Eval. Time, s	2.006	0.819	2.034	0.898	3.104	0.867
NEQLU Time, s	0.136	0.143	0.156	0.136	0.262	0.263
No. of Eqs.	36	36	36	36	54	54
Equivalent No. of Sequential Iter.	45	25	47	27	60	28

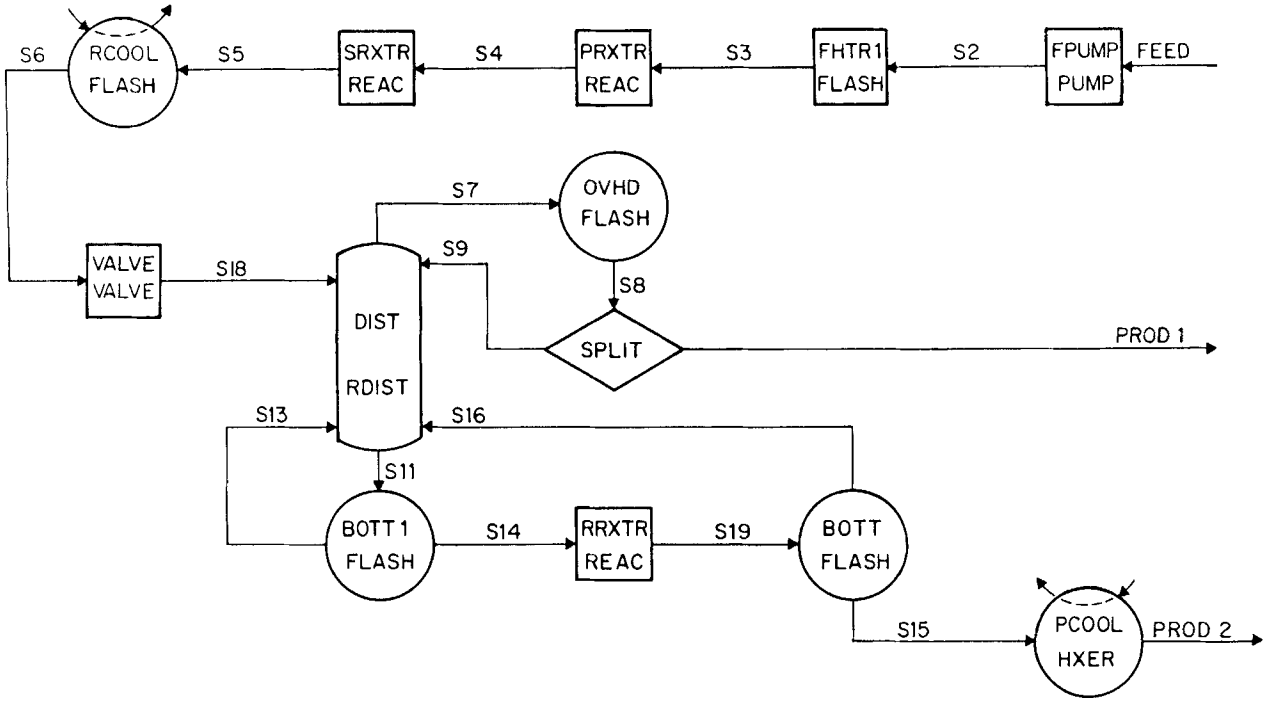

Figure 2. Block diagram for cyclopentadiene recovery process (Problem 2).

the calculated heat load matches the specified value. The result of this case is shown as run 5 in Table 3. In this case, the number of iterations remain at four but the total CPU time increases by about 300%. This result indicates that it is more efficient to include design specifications directly, as in the simultaneous-modular approach, than to use control loops as in the sequential-modular approach. This result is not surprising; for instance, similar results have been reported by Metcalfe and Perkins (1978).

TABLE 6. PROBLEM SPECIFICATIONS FOR CYCLOPENTADIENE RECOVERY PROCESS

Stream	FEED:	Temperature 311.1 K			
		Pressure 0.793 MPa			
		Component flow rates in kgmol/s:			
	CPD	TP	IP	DCY	COD
	0.00386	0.00189	0.00013	0.01232	0.0
FPUMP	Pump; Outlet pressure = 0.862 MPa				
FHTR1	Fired heater; Outlet temperature = 363.3 K				
PRXTR	Adiabatic reactor				
	2CPD → DCP				
	92.5% conversion of CPD				
	Heat of reaction = −75.08 MJ/Kgmole CPD				
PRXTR	Isothermal reactor				
	CPD + TP → COD				
	7.5% conversion of TP				
RCOOL	Water cooler; Outlet temperature = 388.9 K				
VALVE	valve; Outlet pressure = 0.1724 MPa				
DIST	Distillation tower				
	4 ideal stages (no condenser or reboiler)				
	S9 enter stage 1, S18 enter stage 2				
	S13 and S16 enter stage 4				
	Column pressure = 0.1724 MPa				
OVHD	Total condenser				
TSPLT	Splitter; 28.517% of S8 goes to S9				
BOTT1	Partial reboiler; 80% vaporization				
RRXTR	Reactor				
	DCP → 2CPD				
	3% conversion of DCP				
	Heat of reaction = 150.16 MJ/Kgmole DCP				
BOTT	Partial reboiler; 75% vaporization				
PCOOL	Heat exchanger				
	Heat transfer coefficient = 2.834E-4 MJ/s/m^2/K				
	Heat transfer area = 3.716 m^2				

Table 5 shows the performance of SIMMOD with different tear sets. It is clear that the simultaneous-modular approach is not sensitive to the tear set used, except of course that the Jacobian evaluation time for the direct difference approximation case increases proportionally to the total number of tear variables. This can be compared to the results for the sequential-modular simulator FLOWTRAN presented by Rosen and Pauls (1977), who use a Wegstein convergence block with delay. They found that if acceleration was applied on the tear sets {*R*1, *R*2, *R*3} or {Z1, Z2} at every iteration, their program would not converge. If acceleration was applied only every 4th iteration to {*R*1, *R*2, *R*3}, their program would converge in 23 iterations. If acceleration was applied only every 5th iteration to {Z1, Z2}, their program would converge in 48 iterations but in an irregular manner. Comparing our results to these, we can see that because of the large overhead in evaluating the Jacobian, the simultaneous-modular approach is not competitive in this problem if the Jacobian is evaluated by direct difference approximation, even though it requires far fewer flowsheet-level iterations. However, if the Jacobian is calculated by full-block perturbation, then the simultaneous-modular approach compares very well with the sequential-modular approach.

PROBLEM 2: CYCLOPENTADIENE RECOVERY PROCESS

As shown in the last problem, the simultaneous-modular approach converges very rapidly to the solution, but its efficiency is reduced significantly by the amount of work involved in calculating a single Jacobian. One of the reasons for this is that, at least when using the direct difference approximation, the calculation does not take advantage of the fact that during the Jacobian

TABLE 7. PERFORMANCE OF SIMMOD ON MAJOR IRREDUCIBLE BLOCK OF CYCLOPENTADIENE RECOVERY PROCESS

	Run Number					
	1	2	3	4	5	6
Jacobian Eval. Option Used	Direct	Full	Diag.*	Direct	Full	Diag.*
Simple Thermo. Models Used?	Yes	Yes	Yes	No	No	No
Initialization Time, s	1.017	1.002	1.034	0.998	1.010	1.009
Simultaneous Iterations	2	2	10	2	2	10
Function Eval. Time, s	0.389	0.368	1.265	0.395	0.358	1.260
Jacobian Eval. Time, s	1.052	0.419	0.209	1.441	0.829	0.284
NEQLU Time, s	0.028	0.028	0.088	0.030	0.027	0.095
Equiv. No. of Sequential Iter.	14	9	16	17	13	17

Tear set generated by SIMMOD is {S9,S11}.
Number of equations = 14.
Major irreducible block consists of the following units: BOTT1, RRXTR, BOTT, DIST, OVHD, TSPLT.
* Full-block perturbation was used on the REAC units.

evaluation, the modules are solving a series of slightly different problems. In this example, we look at some techniques for increasing the efficiency of Jacobian evaluation.

The second test problem is the cyclopentadiene recovery process from the CHESS manual (Motard and Lee, 1973). The block diagram of this problem is shown in Figure 2 and the specifications for this problem are given in Table 6. This process was modeled by 10 modules and 18 streams. The sequential-modular simulator CHESS took 22 iterations to converge this problem using bounded Wegstein.

For this problem, the CPU time is dominated by the distillation calculation. In our implementation of the rigorous distillation module, two simple techniques are used to reduce the flowsheet-level Jacobian evaluation time:

1. The Jacobian matrix used in the distillation calculation is saved on disk and used for subsequent calculations. This allows the efficient solution of slightly different distillation problems, whether they are performed consecutively, as in the case of block perturbation, or nonconsecutively, as in the case of direct difference approximation. Of course for the nonconsecutive direct difference approximation calculations, more disk I/O operations will be required since the matrix will have to be saved on disk several times, while for the consecutive block perturbation calculations the matrix must be saved only once. This technique will result in a significant savings when the direct difference approximation is used, but when block perturbation is used there will be no significant savings unless more than one Jacobian evaluation is required per problem or unless a parametric study is being performed and several similar simulation problems are being solved.

2. An option is included to use simple thermodynamic property models for distillation calculations during the flowsheet-level Jacobian evaluation. The idea of using simplified thermodynamic models to reduce the computation time and/or to avoid the problem of composition dependency has been employed by several others (e.g., Billinsley, 1970; Boston and Sullivan, 1974; Hutchison and Shewchuk, 1974). In this case we use the Peng-Robinson equation of state to generate constants in the following simple models:

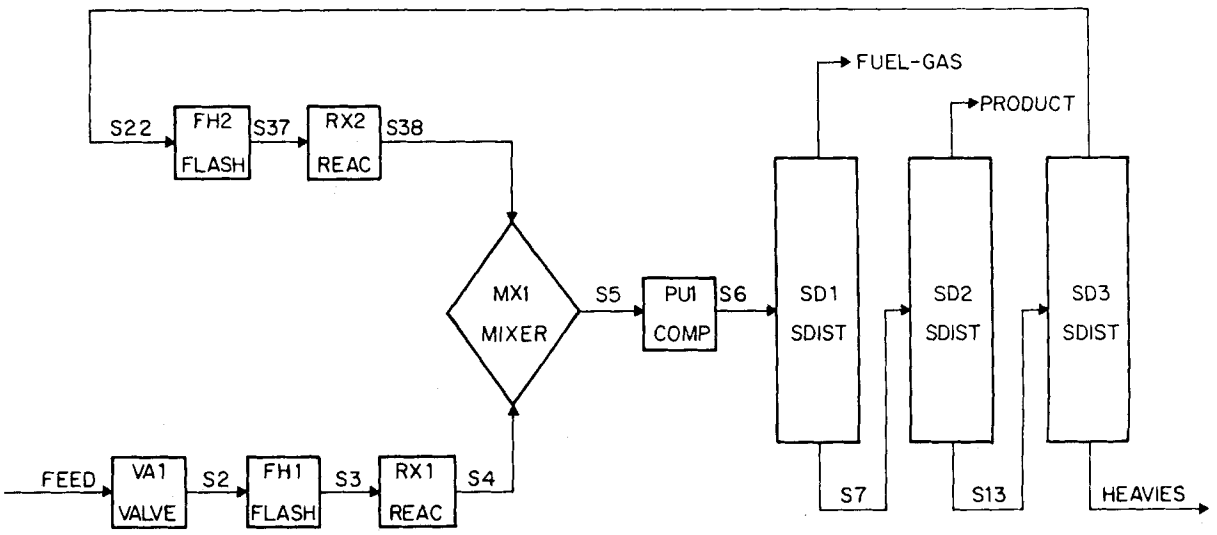

Figure 3. Block diagram for simple ethylene plant (Problem 3).

TABLE 8. PROBLEM SPECIFICATIONS FOR SIMPLE ETHYLENE PLANT

Stream	FEED:	Temperature	294.4 K
		Pressure	4.137 MPa
		Component flow rates:	
		Ethane	0.01008 kgmol/s
		Propane	0.01512 kgmol/s
VA1	Valve		
	Outlet pressure = 0.620 MPa		
FH1	Fired heater		
	Outlet temperature = 344.44 K		
	Pressure drop = 0.069 MPa		
RX1	Isothermal reactor		
	$3C_2H_6 + 6C_3H_8 \rightarrow 4H_2 + 4CH_4 + 5C_2H_4 + 2C_3H_6 + C_4H_{10}$		
	90% conversion of C_3H_8		
MX1	Mixer		
PU1	Compressor		
	No. of compression stages = 3		
	Outlet pressure = 4.137 MPa		
SD1	Simple distillation		
	Take 100% H_2 and CH_4 overhead		
SD2	Simple distillation		
	Take 99% C_2H_4 and 5% C_2H_6 overhead		
FH2	Fired heater		
	Outlet temperature = 344.44 K		
	Pressure drop = 0.069 MPa		
RX2	Isothermal reactor		
	$4C_2H_6 \rightarrow 2H_2 + 2CH_4 + 3C_2H_4$		
	80% conversion of C_2H_6		

$$\ln(K_{ij}P) = A_{ij} + B_{ij}/T$$

$$HDEP_j^L = A_j^L + B_j^L T$$

$$HDEP_j^V = A_j^V + B_j^V T,$$

where i is the component number, j is the stage number, and the $HDEP$'s are enthalpy departures per unit mass. These simple composition-independent models are then used to generate an approximate Jacobian for the flowsheet level.

The following irreducible blocks were identified by SIMMOD: (FPUMP), (FHTR1), (PRXTR), (SRXTR), (RCOOL), (VALVE), (BOTT1, RRXTR, BOTT, DIST, OVHD, TSPLT), (PCOOL). The tear set {S9, S11} was identified for the only nontrivial block. The performance of the simultaneous-modular approach on this test problem is shown in Table 7. These comments are in order:

1. The number of components in this problem is 5, so each stream represents 7 variables, and each stream connection equation represents 7 equations.

2. The number of distillation calculations required to calculate the Jacobian by direct difference approximation, full-block perturbation and diagonal-block perturbation are respectively 15, 22, and 4.

3. The Jacobian evaluation time for the direct difference approximation case is longer than the full-block perturbation case, even though about 30% fewer distillation calculations are required. This is because of the I/O time involved in saving and retrieving intermediate results.

4. When the Jacobian is calculated by diagonal-block perturbation, the Jacobian evaluation time is very short, but the simultaneous-modular approach requires many more iterations to converge the problem. This is because a poor approximation of the Jacobian is generated.

Comparing these results to the 22 iterations required by CHESS, we can see that the simultaneous-modular approach compares well with the sequential-modular approach on this problem. This is because the Jacobian evaluation time is not excessive. Also comparing runs 1–3 to runs 4–6, we can see that when simple physical property models are employed during the flowsheet-level Jacobian evaluation, the Jacobian evaluation time is reduced and the convergence is not affected.

TABLE 9. PERFORMANCE OF SIMMOD ON MAJOR IRREDUCIBLE BLOCK OF SIMPLE ETHYLENE PLANT

	Run Number		
	1	2	3
Jacobian Eval. Option Used	Direct	Full	Diag.*
Initialization Time, s	0.244	0.239	0.244
Simultaneous Iterations	2	2	2
Function Eval. Time, s	0.253	0.255	0.254
Jacobian Eval. Time, s	0.830	0.490	0.201
NEQLU Time, s	0.020	0.021	0.020
Equiv. No. of Sequential Iter.	24	17	11

Tear set generated by SIMMOD is {S38}.
Number of equations = 9.
Major irreducible block consists of the following units: MX1, PU1, SD1, SD2, SD3, FH2, RX2.
* Full-block perturbation was used on RX2.

PROBLEM 3: SIMPLE ETHYLENE PLANT

The third test problem is the simple ethylene process from CHESS example 3. The block diagram of this problem is shown in Figure 3 and the specifications for this problem are shown in Table 8. The sequential-modular simulator CHESS took only 6 iterations to converge this problem using bounded Wegstein. This problem was included to show that the sequential-modular approach may be still preferred for simple problems like this.

The following irreducible blocks were identified by SIMMOD: (VA1), (FH1), (RX1), (MX1, PU1, SD1, SD2, SD3, FH2, RX2). Stream S38 was identified as the only tear stream. The performance of the simultaneous-modular approach with different options for calculating the Jacobian is shown in Table 9. This problem is linear, thus the program finds the solution in one iteration, but it performs one extra iteration to confirm it. However, while the simultaneous-modular approach is certainly competitive with the sequential-modular approach on this problem, it still requires more CPU time than the sequential-modular approach because of the overhead involved in the Jacobian evaluation. This result suggests that since both the sequential-modular and simultaneous-modular approaches can be implemented using the same set of modules, it may be desirable to maintain a sequential-modular option within the overall framework of a simultaneous-modular program.

PROBLEM 4: RAW PRODUCT RECOVERY SECTION OF A NATURAL GASOLINE PLANT

The fourth problem is the raw product recovery section of a natural gasoline plant, from CHESS example 4. The flow diagram of this problem is shown in Figure 4. Complete specifications for this problem and a sample input file for SIMMOD are given by Chen (1982). This problem is the largest test problem in the CHESS manual, and it is also one of the largest test problems available in the literature. From Chen (1982) however one can see that even for a problem of this size the input file is still

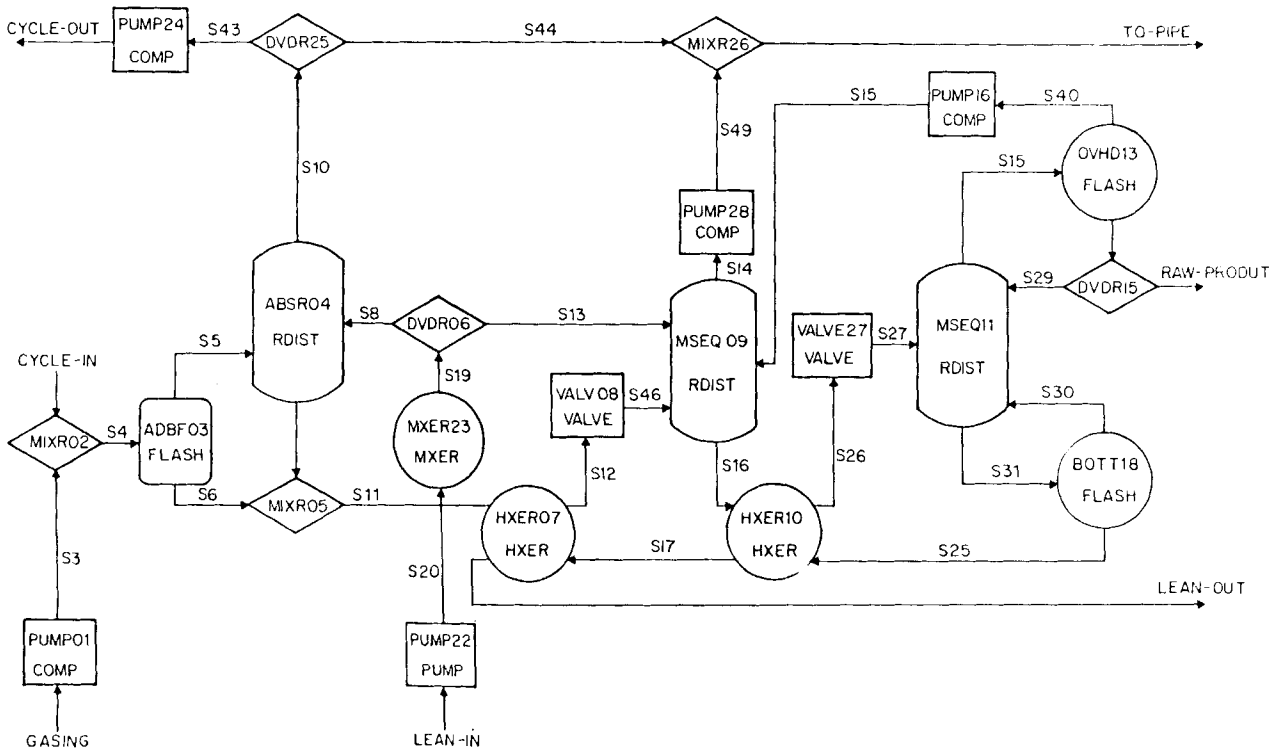

Figure 4. Block diagram for raw product recovery section of a natural gasoline plant (Problem 4).

relatively simple (63 noncomment lines). The sequential-modular simulator CHESS did not find the solution in 40 iterations, using bounded Wegstein.

This problem consists of 22 modules and 38 streams. The only nontrivial irreducible block consists of (HXER07, VALV08, MSEQ09, HXER10, VALV27, MSEQ11, BOTT18, DVDR15, OVHD13, PUMP16). The tear set {S16, S29, S31} was identified by SIMMOD. It can be easily verified that this tear set has the minimum number of tear streams and that each recycle loop is torn only once. The performance of the simultaneous-modular approach is shown in Table 10. These comments are in order:

1. In the three sequential iterations used for initialization, the average time per iteration is about 3.6 s. However, if we determine the average sequential iteration time from the function evaluation time the result is only about 0.8 s. The major reason for the difference in CPU time is because in the first few iterations, the inputs to the distillation module are such that despite many iterations within the distillation module, no solution for the distillation calculations can be found. It should be mentioned that this problem can be alleviated by supplying better initial values for tear variables.
2. Using the Jacobian calculated by diagonal-block perturba-

TABLE 10. PERFORMANCE OF SIMMOD ON MAJOR IRREDUCIBLE BLOCK OF RAW PRODUCT RECOVERY SECTION OF NATURAL GASOLINE PLANT

	Run Number					
	1	2	3	4	5	6
Jacobian Option Used	Direct	Full	Diag.	Direct	Full	Diag.
Simple Thermo. Models Used?	Yes	Yes	Yes	No	No	No
Initialization Time, s	10.686	10.412	10.823	11.010	10.896	10.979
Simultaneous Iterations	14	8	30	12	13	28
Function Eval. Time, s	12.704	6.652	17.502	9.686	11.092	12.140
Jacobian Eval. Time, s	5.516	3.272	1.054	11.939	8.855	1.820
NEQLU Time, s	0.331	0.226		0.293	0.315	
Equiv. No. of Sequential Iter.	27	18		35	31	

Tear set generated by SIMMOD is {S16,S29,S31}.
Number of equations = 36.
Major irreducible block consists of the following units: BOTT18,HXER10,VALV27,MSEQ11,OVHD13,DVDR-15,PUMP16,HXER07,VALV08,MSEQ09.

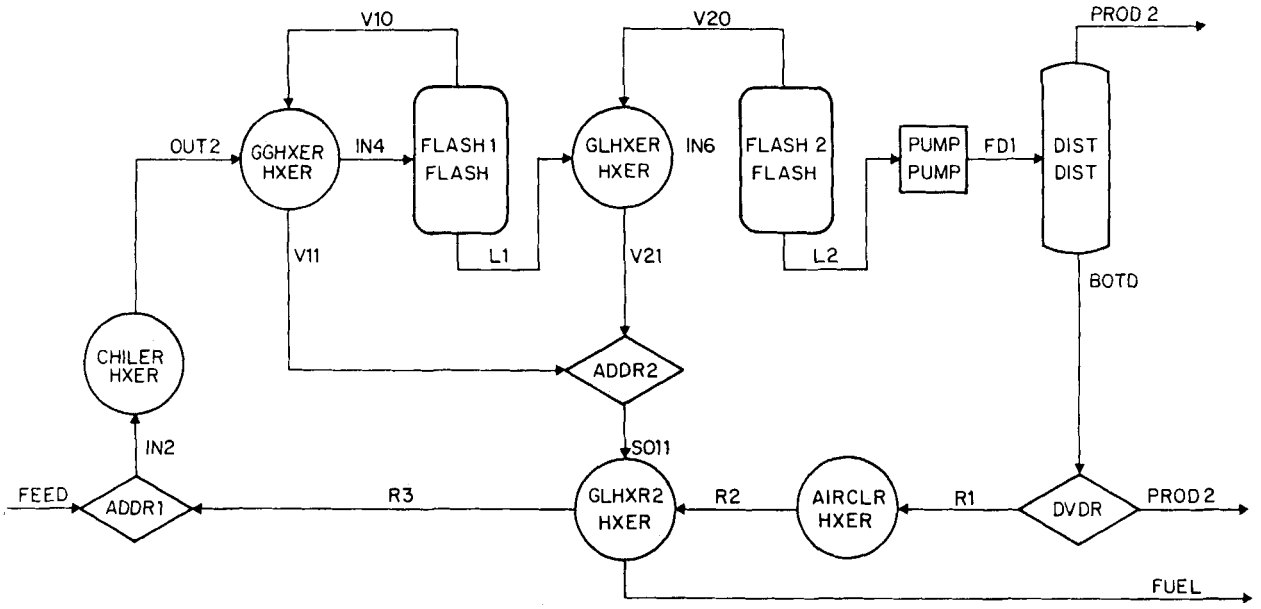

Figure 5. Block diagram for light hydrocarbons recovery process (Problem 5).

tion (runs 3 and 6), the simultaneous-modular approach failed to solve the problem.

3. Comparing runs 1–2 to runs 4–5, we can see that using simple thermodynamic models in evaluating the flowsheet-level Jacobian significantly reduces the Jacobian evaluation time and makes the simultaneous-modular approach more competitive.

4. Run 1 required two more iterations than run 4. This is probably because the results calculated using the simple thermodynamic models were passed downstream to other modules when the Jacobian was calculated by direct difference approximation, thus creating some inconsistencies.

5. Run 2 required 5 fewer iterations than run 5. This is probably because it is easier to converge the distillation calculation when composition-independent simple thermodynamic models are used. As a result, a more consistent Jacobian was obtained.

This problem clearly demonstrates that the simultaneous-modular approach is capable of handling more difficult problems than the sequential-modular approach, if a reliable method such as the modified Powell's method (Chen and Stadtherr, 1981) used by NEQLU is employed to solve the flowsheet-level nonlinear equations, and if a good approximation of the Jacobian is used in the calculation.

PROBLEM 5: LIGHT HYDROCARBONS RECOVERY PROCESS

The last problem is a light hydrocarbons recovery process. The block diagram of this problem is shown in Figure 5 and the complete specifications for this problem are given by Chen (1982). This problem is exercise 25 in the FLOWTRAN exercise book (Clark, 1977). As noted by Clark, even when starting with good initial estimates, and using bounded Wegstein, FLOWTRAN still requires "many" iterations to converge this problem.

The tear set {*R*3, *V*10, *V*20} was identified by SIMMOD. It can be easily verified that this tear set has the minimum number of tear streams and that each recycle loop is torn only once. The performance of the simultaneous-modular approach is shown in Table 11. These comments are in order:

1. Using all three options for calculating the Jacobian, the simultaneous-modular approach solved this problem in three simultaneous iterations, without using a good initial estimate.

2. The diagonal-block perturbation technique works surprisingly well on this problem. We have no particularly satisfying explanation to offer for this.

3. The Jacobian evaluation time for the direct difference approximation case is excessive.

Again this problem demonstrates that the simultaneous-modular approach seems at least as reliable as the sequential-modular approach, if not more so.

CONCLUDING REMARKS

Based on the results presented above, we can make the following conclusions about the performance of the simultaneous-modular approach on process simulation or controlled simulation problems:

1. With a good method for solving the flowsheet-level nonlinear equations, and an accurate approximation of the flowsheet-level Jacobian, the simultaneous-modular approach seems at least as reliable as the sequential-modular approach.

TABLE 11. PERFORMANCE OF SIMMOD ON LIGHT HYDROCARBON LIQUIDS RECOVERY PROCESS

	Run Number		
	1	2	3
Jacobian Option Used	Direct	Full	Diag.
Initialization Time, s	0.548	0.547	0.548
Simultaneous Iterations	3	3	3
Function Eval. Time, s	0.849	0.866	0.836
Jacobian Eval. Time, s	7.568	3.530	0.719
NEQLU Time, s	0.118	0.114	0.095
Equiv. No. of Sequential Iter.	44	24	11

Tear set generated by SIMMOD is {R3,V10,V20}.
Number of equations = 30.

2. The relative merits of the three options for calculating the Jacobian are:
   a. Calculating the Jacobian by diagonal-block perturbation is not recommended for a general-purpose implementation, because it may take more iterations to converge (Problem 2), or it may fail (Problems 1 and 4), although sometimes it works surprisingly well (Problems 3 and 5).
   b. Calculating the Jacobian by direct difference approximation gives reliable convergence, but the Jacobian evaluation time may be excessive. This problem would become even more severe with increasing problem size and/or complexity.
   c. We recommend that the Jacobian be calculated by full-block perturbation. It is reliable, the Jacobian evaluation time is moderate, and it will remain so even with increasing problem size and/or complexity.
3. When the Jacobian is calculated by full-block perturbation, the simultaneous-modular approach is competitive to or sometimes much better than the sequential-modular approach in terms of computational efficiency. Also it is expected that in the following circumstances the advantages of the simultaneous-modular approach would be even greater:
   a. In a parametric study a series of problems for the same process under slightly different conditions is solved. If the flowsheet-level Jacobian is saved from one problem to the next, there would be no Jacobian evaluation expense nor initialization expense, and the NEQLU overhead would be very small. Thus the number of equivalent sequential-modular iterations will generally approach very closely the number of simultaneous iterations, which in this case is typically two or three. The sequential-modular approach may solve some parametric simulation problems in only two or three iterations, while for other problems five or six, or occasionally more may be required. In the latter instance the simultaneous-modular approach offers a significant advantage, especially if the number of cases to be solved is large. Such an advantage will be more dramatic on parametric design or optimization problems.
   b. As shown in Problem 1, when there are design specifications to be accounted for, including them directly on the flowsheet level, as in the simultaneous-modular approach, can be much more efficient than using control loops, as in the sequential-modular approach.
   c. If the equations describing a unit are solved by a simultaneous linearization approach in the corresponding module, then determining the input-output relationships for the module would only involve the solution of a few systems of linear equations, each with the same coefficient matrix. As was discussed previously (Chen and Stadtherr, 1985a) this menas that the Jacobian could be found analytically, eliminating the need for block perturbation and decreasing the time needed to compute the Jacobian.
   d. When simple thermodynamic models are used during flowsheet-level Jacobian evaluation, the Jacobian evaluation time can also be significantly reduced, as shown in Problems 2 and 4.
4. The use of different tear sets has very little effect on the convergence of the simultaneous-modular approach. This is to be expected, as can be seen by considering a linear problem. In this case the performance of the sequential-modular approach may vary with the choice of tear set, while the simultaneous-modular approach with an exact Jacobian will find the solution in just one iteration using any tear set.

In Part III of this series, we study the performance of the simultaneous-modular approach on process optimization problems, and present the results of numerical experiments comparing different computational strategies for the optimization problem.

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NOTATION

A_{ij}, B_{ij} = constants in simple model for K_{ij}
A_j^L, B_j^L = constants in simple model for $HDEP_j^L$
A_j^V, B_j^V = constants in simple model for $HDEP_j^V$
$HDEP_j^L$ = liquid enthaply departure per unit mass for stage j
$HDEP_j^V$ = vapor enthalpy departure per unit mass for stage j
K_{ij} = equilibrium vaporization factor for component i on stage j
NI_{SIM} = number of simultaneous-modular iterations
P = pressure
T = temperature

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