A STUDY OF THE CONVENIENCE OF THE SIMULTANEOUS AND THE SEQUENTIAL APPROACH FOR SIMULATION OF SOME TYPICAL CHEMICAL PROCESSES

V.Vašek[a], J.Klemeš[a], Č.Vermouzek[b] and M.Dohnal[b]

[a] *Research Institute of Chemical Equipment, Department of Applied Mathematics, 602 00 Brno and*

[b] *Department of Mechanical Equipment of Chemical and Food Plants, Technical University, 611 00 Brno*

Received June 6th, 1973

Two approaches are compared in the paper to the problem of simulation of complex steady-state chemical processes: *a*) A simultaneous approach based on a modified Nagiev's method solving the whole part of the process containing recycles simultaneously, and, *b*) a sequential approach requiring the study of the process topology, *i.e.* decomposition and localization of the recycles. The comparison is made by the SIPRO programming system. The efficiency of the two approaches is examined in terms of the computer time based on experience with process design gathered in the course of solving various typical technological problems.

Digital computer-aided simulation of chemical processes is an extraordinarily important part of the design work of a number of leading process design institutions. Various simulation algorithms capable of practical utilization have been existing[1,2]. Yet, the question of the convenience of various simulation algorithms for different types of chemical processes remains unsolved.

The simulation methods can be roughly divided into two groups depending on whether they do or do not call for decomposition.

Algorithms involving decomposition are termed sequential, *e.g.* Pacer[3]; the latter group is based on principles outlined by Nagiev[4]. From the viewpoint of the computing time the choice of the method is extremely important. Certain papers dealing with this topics[3,5] have appeared in the literature over the last decade.

The most extensive work in this respect is that of Umeda and Nishio[6]. The authors analyzed three simulation methods using two relatively simple processes. Their study, of course, does not compare the methods but definite computer programs. General advantages and drawbacks of the two methods thus combine with the quality of computer programming, not to speak about possible modifications of both methods.

This paper makes use of the experience gathered in the course of solving a number of problems by the Sipro programming system[7] using computer DATASAAB D21. This system contains algorithms formulated on the basis of both approaches and an attempt was made to generalize this experience.

Simultaneous and Sequential Algorithms

The algorithm utilizing the simultaneous method originated as a modification of the approach published by Nagiev and was further arranged by Rosen[8]. The term of the recycle fraction of a component t going from the i-th node into the j-th one is introduced as follows

$$\alpha_{ij}^t = S_{ij}^t / \lambda_i^t , \tag{1}$$

where the total flow rate of the component t through the node i is defined as

$$\lambda_i^t = \sum_{j=1}^{K} S_{ji}^t \tag{2}$$

K is the number of process units (nodes) and S_{ij}^t is the flow rate of the component t between node i and j. The node number 0 represents the system surroundings.

With the aid of the recycle fractions the balance equations for the component t are

$$\begin{aligned}
(1 - \alpha_{11}^t)\lambda_1^t - \alpha_{12}^t\lambda_2^t \quad - \ldots - \alpha_{1K}^t\lambda_K^t &= S_{0,1}^t \\
-\alpha_{21}^t\lambda_1^t + (1 - \alpha_{22}^t)\lambda_2^t - \ldots - \alpha_{2K}^t\lambda_K^t &= S_{0,2}^t \\
\vdots \\
-\alpha_{K1}^t\lambda_1^t - \alpha_{K2}^t\lambda_2^t - \ldots + (1 - \alpha_{KK}^t)\lambda_K^t &= S_{0,K}^t .
\end{aligned} \tag{3}$$

The calculation rests on a repeated solution of the set of linear equations in K unknowns, Eq. (3), for all F balanced components. In cases where the recycle fractions can be given in advance and remain constant the balance equations need be solved for each component only once. Generally, however, the recycle fractions are described by equations representing mathematical models of the process units (apparatuses). In these equations, which may be of very different nature, appear as independent variables the flow rates of the balanced quantities through the nodes which are not known in advance and vary in the course of the computation. Accordingly, the values of the recycle fractions in the output streams belonging to such nodes cannot be given.

A more detailed description of the simultaneous algorithm used in Sipro has been published elsewhere[9].

A basic idea of the sequential method is to iterate a minimum number of quantities simultaneously. Prior to the calculation proper it is therefore necessary to decompose (tear) the flow sheet graph, localize recycles and specify a precedence-ordering of the process units and the branches in which the streams specifications must be estimated and checked. According to this strategy the computation is repeated until the stream variables in the checked branches in two succesive iterations differ by less than some prescribed tolerance. One iteration represents recalculation of all process units[10].

Comparing the computing time needed to solve the simulation problem by both methods the following inferences can be drawn: The simultaneous algorithm requires no time for decomposition but it calls for a solution of the set of linear balance equations in each iteration in addition to the calculation of the mathematical models of the process units. The sequential algorithm involves decomposition but in subsequent iteration solves only the mathematical models of the process units.

Both algorithms have the same models of the apparatusses as well as other subprograms (subroutines to evaluate physico-chemical data, reading the input data, the printout *etc.*)[11]. Let us assume that for a simulation of identical processes the two algorithms compared will require the same number of iterations. This will assist in explaining certain relations. The analysis shows the computing time to depend on the following quantities:

The number of nodes (process units) involved. The simultaneous method necessitates solution of the set of linear equations and with the aid of some standard method (*e.g.* the Gauss elimination or its modifications) the number of operations and hence the computer time grows approximately with the third power of the number of nodes (Fig. 1). However, the matrix of the set of equations contains many zero elements and a somewhat modified Gauss elimination method of solution was therefore used. The computational effort required by this method also depends on the number of the nodes and branches (Fig. 1) but it is less.

Increasing number of nodes increases also the time of decomposition. The dependence though is not so unambiguous because of the effect of various complexity of the process flow sheet.

The number of streams involved. The effect on the simultaneous method becomes manifest only when using the modified Gauss elimination; the effect on the sequential method is analogous to that of the number of the nodes.

The structure of the process. The complexity of the process flow sheet, *i.e.* the number of all possible interstreams between individual nodes, has no substantial effect on the simultaneous method but it affects decisevely the decomposition time of the sequential method. If, for instance, the process flow sheet consists of a tree or a single loop, then either no decomposition or only a relatively short one is necessary. It is so because of a relatively small number of interstreams. In case of a more complex flow sheet graph the time of decomposition may become a manifold of the previous one even with the same number of nodes.

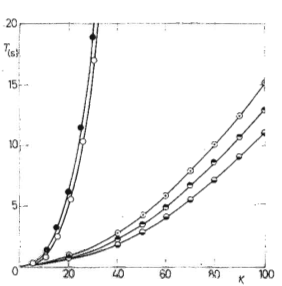

FIG. 1

Computer Time T as Function of Number of Nodes K

● Gauss elimination method, ○ Crout's method, ◓ Modified Gauss elimination, the flow sheet graph with $2(K-1)$ streams acyclic, ⊙ Modified Gauss, the flow sheet graph with $2(K-1)$ streams cyclic, ◒ Modified Gauss, the flow sheet with $K-1$ streams.

The number of components. Each iteration in the simultaneous algorithm poses a solution of the set of F linear equations. On the other hand, the time for decomposition is not a function of the number of iterations.

These relations may be demonstrated on the following example: Consider a process symbolized by the graph in Fig. 2. Decomposition of the flow sheet by the Sipro system took 321 s. The time needed in a single iteration to solve the set of the balance equations was 1·85 s. The plot of the computer time *versus* the number of iterations for the simultaneous algorithm is shown in Fig. 3. The time of decomposition is indicated by the dashed line. The time of solving the mathematical models is the same for both algorithms and was not therefore included. From Fig. 3 it is apparent that for a small number of components the simultaneous algorithm is more convenient. With growing number of the components, however, the time for the solution of the set of balance equations exceeds that of decomposition after already a few iterations.

The above considerations, however are hypothetical because for a majority of processes the convergence of both routines and hence the number of iterations for both

TABLE I

Classification of Process Flow Sheets According to Various Aspects

Linearity	Number of nodes	Number of recycles
Linear	up to 10	0
Non-linear in energy balance	11—25	1—3
Non-linear in material balance	<25	>3

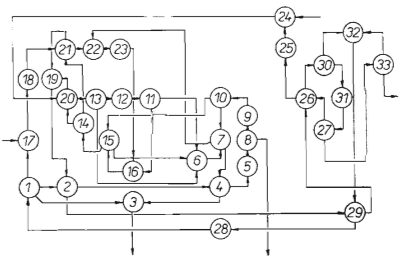

FIG. 2

Process Flow Sheet with 33 Nodes, 53 Streams and 19 Recycles Loops

methods compared will be different. The number of iterations is affected by the size of the simulated process, the structure of the process flow sheet, the types of process units as well as the information necessary for estimation and the choice of suitable models of the process units[12].

It is thus very difficult to assess which of the methods is more efficient. An attempt was therefore made to analyse at least certain extreme types of the processes and to assign suitable algorithms. All processes are divided according to the aspects summarized in Table I.

Analysis of the Solutions of Individual Types of Processes

a) If all nodes and balanced components can be assigned their recycle fractions, the simultaneous method has a considerable advantage. The set of balance equations is solved only once for each component, the calculation does not require iteration and it is highly accurate. For the sequential method, on the contrary, it is necessary (if the process has recycles) to iterate even in such case and, moreover, to decompose. The number of iterations depends on the required accuracy.

Let us examine three examples of chemical processes, all parts of a deoiling and dewaxing plant. The first, solvent regeneration (Fig. 4), contains no recycle loops and the sequential method needs no decomposition or only a very simple one. A comparison in the form of the simultaneous/sequential method ratio gives: The number of iteration 1/1, time of decomposition 0/0, time of simulation 10·5/8, total time 10·5/8 (all times in seconds). The second example is a medium size process with three recycles (Fig. 5). As it is apparent from the following results the simultaneous method is more effective but the difference is from practical standpoint negligible. The simultaneous/sequential method ratios are: The number of iterations 1/6,

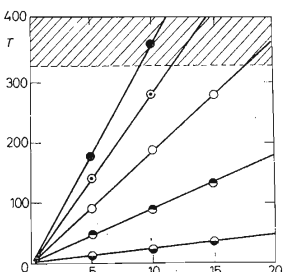

FIG. 3

Computer Time *T versus* Number of Iterations *N* for Problem in Fig. 2 by Simultaneous Method

The time of tearing is shown by dashed line; shaded area indicates region where the sequential method is more efficient. ● 20, ⊙ 15, ○ 10, ◓ 5, ◒ 1.

time of decomposition 0/91, time of simulation 8·5/35, total time 8·5/125. Finally, as the third example, the whole deoiling and dewaxing plant (Fig. 6). The results for this complex process with 77 nodes, 116 streams and more than 600 recycle loops given again as the ratios of the two methods indicate clearly the superiority of the simultaneous method: The number of iterations 1/12, time of decomposition 0/1675, time of simulation 72/363 and the total time 72/2038.

The results furnish following conclusions: In cases when the recycle fractions for all balanced quantities can be specified it is advantageous to use the simultaneous method. The calculation is performed accurately (the numerical error is that of the solution of the set of linear equations) and without iteration. The computer time is either smaller than that by the sequential method or the difference is practically insignificant.

b) The picture will be different if the recycle fractions cannot be given for one of the components – the thermal energy. For processes without recycles the sequential method is then substantially better because the calculation proceeds without iteration, node by node. The results of the computation of the process shown schematically in Fig. 4, assuming that the recycle fractions for heat are unknown, in the form of the ratios of the two methods are: The number of iterations 8/1, time of decomposition

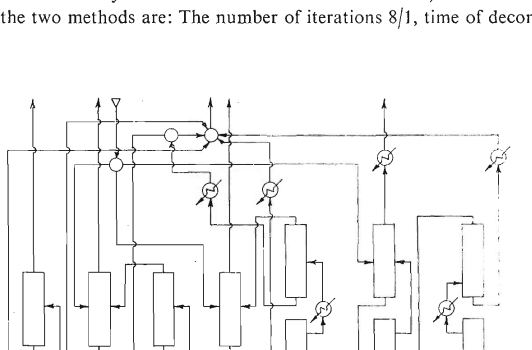

FIG. 4

Medium Size Process Flow Sheet without Recycle Loops (solvent recovery as a part of oil and wax removal unit)

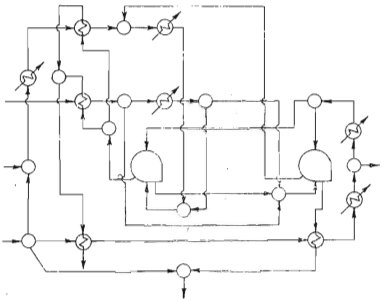

FIG. 5
Medium Size Process Flow Sheet with Three Recycle Loops

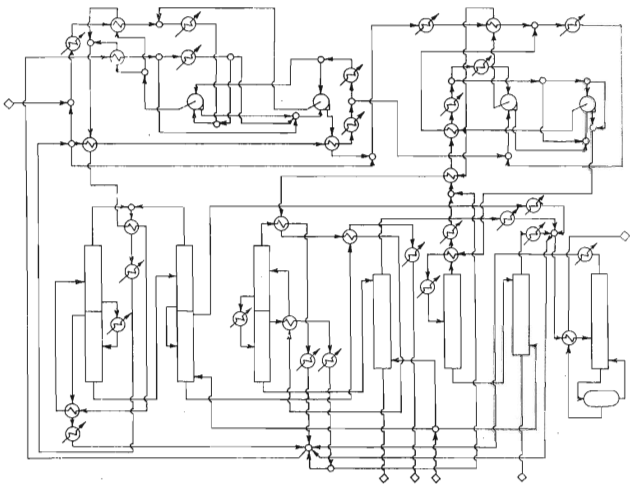

FIG. 6
Extensive Process Flow Sheet with More than 300 Recycle Loops

0/0, time of simulation 363/43, total time 363/43. The simultaneous method calls for a few iterations involving solution of the heat balances in each of them. Processes containing one or more recycles necessitate iteration in any of the two methods. The simultaneous method has an edge over the other in that it iterates only one component while the other (material) balance is solved in an non-iterative fashion. The sequential method calls for decomposition. The following results again as the simultaneous/sequential method ratios were achieved in solving the intermediate process (Fig. 5): The number of iterations 8/8, time of decomposition 0/118, time of simulation 199/184, total time 199/302. It is seen that although the number of iterations is the same, the total time of the simultaneous method is shorter. The increase of the total time for the sequential method was caused by decomposition. In case of a relatively extensive process (Fig. 7) the situation is analogous. Despite of the results obtained no unambiguos conclusion regarding the relative efficiency of the two methods can be offered because of the effect of the large number of non-linear process units and the structure of the process flow sheet.

c) The most difficult case occurs when the recycle fractions of all balances components vary. For a process without recycle loops (Fig. 4) the sequential methods is clearly more advantageous. In contrast, the simultaneous method would require iterative solution solving *F*-times the set of linear balance equations in each iteration.

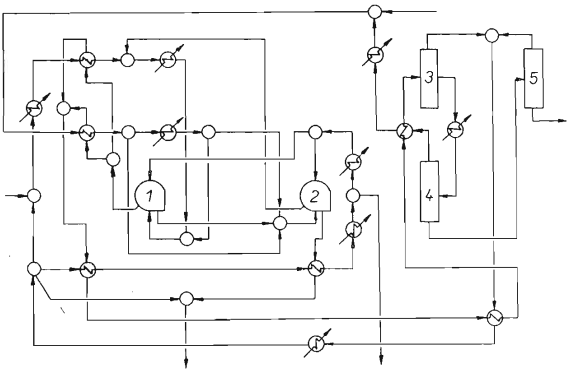

FIG. 7

Process Flow Sheet with 33 Nodes, 53 Streams and 19 Recycles

Cyclic processes are somewhat more complex. The number of iterations is strongly affected by the initial guess. For the sequential method one has to estimate the flow rate of balanced components in several streams. The number of such streams is minimized by the tearing program. The simultaneous method requires estimate of the recycle fractions, or the amount of exchanged heat for non-linear model of the process units. A comparison of both methods is based on the assumption that all estimated variables are equivalent as to the labouriousness of the estimate and the effect on the iterative computation. With this simplification as more efficient would appear the method iterating fewer quantities.

Example: Fig. 8 shows the flow sheet graph of a process consisting of 5 non-linear process units and a single linear one. Owing to the structure of the graph only F values need be estimated for the sequential method; Q values for the simultaneous method

$$Q = \sum_{i=1}^{N} (l_i - 1)\, F, \qquad (4)$$

where F is the number of balanced quantities and l_i is the number of output streams from node i. N designates the number of non-linear process units. 5 . F values must be estimated in case shown in Fig. 8.

In contrast, the flow sheet depicted in Fig. 9 has only a single non-linear process unit but the flow sheet is so complex that the sequential methods necessitates estimates in three streams. For this reason F values must be estimated for the simultaneous and 3 . F values for the sequential method. Let us note still that if the single non-linear process unit is non-linear only thermally the simultaneous method calls for the estimate of only one value.

It must be realized that the notion "non-linear process unit", *i.e.* a unit with constant recycle

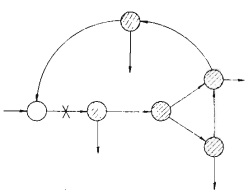

Fig. 8

Process Flow Sheet with 5 Non-Linear and 1 Linear Node

The stream to be estimated in the sequential method is marked by cross.

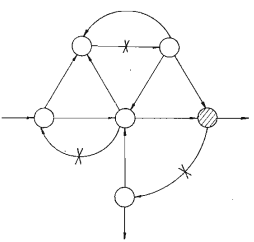

FIG. 9

Process Flow Sheet with 1 Non-Linear and 5 Linear Nodes

The stream to be estimated in the sequential method is marked by cross.

fractions, may represent not only piping but possibly a complex unit operation for which we either assume or wish to retain certain division of the balanced quantities.

As a practical example let us examine a relatively extensive process with 33 nodes, 53 streams and 19 recycle loops (Fig. 7). In the first case we considered the function of the flash distillations (nodes 3, 4, 5) to be known specifying thus the recycle fractions in the output streams. The only non-linear units were the filters (nodes 1 and 2). Under these conditions the results show clearly the simultaneous method to be superior (simultaneous/sequential method ratios): The number of iterations 15/10, time of decomposition 0/4·6, time of simulation 832/521 and the total time 852/937. Considering the flash distillations to be non-linear units the situation is considerably different as indicate the simultaneous/sequential method ratios: The number of iterations 25/12, time of tearing 0/416, time of simulation >1600/637, the total time >1600/1053. Due to the effect large number of quantities that must be estimated for the simultaneous method the number of necessary iterations grows making the problem difficult to solve. The sequential method despite of the relatively tedious tearing handles the problem relatively easily.

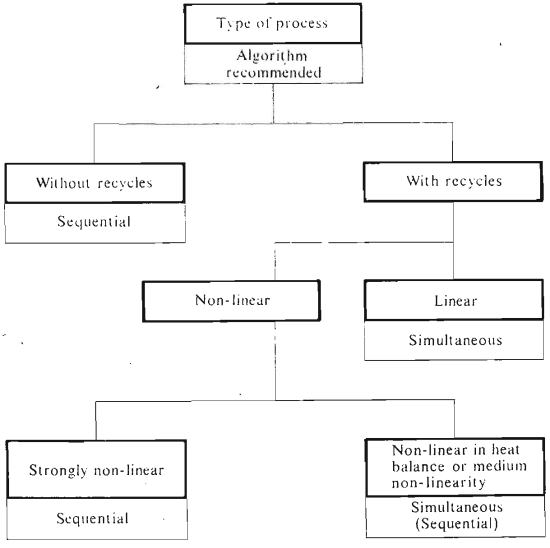

FIG. 10

Convenience of Simulaneous and Sequential Algorithm for Simultation of Various Types of Processes

As it is apparent from the above examples that without decomposing the process flow sheet it is often difficult to ascertain how many values must be estimated if the sequential method is to be applied. For the same reason it is difficult to tell which of the two methods is more efficient. The conclusions can be made only in the form of general recommendations shown graphically in Fig. 10.

The effect was not considered in the paper of various means of acceleration of convergence on the course of the simultaneous method.

REFERENCES

1. Perris F. A.: *User's Description for Flowpack.* Central Instrument Research Laboratory, Imperial Chemical Industries Ltd. 1971.
2. Myles A. F., Chai H. F.: *General Flowsheet Program*, Computer program No PO404. Information Systems Department, M. W. Kelogg Co. 1971.
3. Crowe C. M., Hamielec A. E., Hoffman T. W., Johnson A. I., Woods D. R., Shannon P. T.: *Chemical Plant Simulation.* Prentice-Hall, New York 1971.
4. Nagiev M. F.: *Teoria Recirculacii i Povyšenie Optimalnosti Chemičeskich Procesov.* Nauka, Moscow 1970.
5. Kessler M. G., Griffiths P. R.: Proc. Am. Petrol. Inst. 43, Sec. III, p. 49, 1963.
6. Umeda T., Nishio M.: Ind. Eng. Chem. Proc. Des. Dev. *11*, 153 (1972).
7. Dohnal M., Klemeš J.: Chem. průmysl *21*, 7 (1971).
8. Rosen M. E.: Chem. Eng. Progr. *58*, 10 (1962).
9. Klemeš J., Vašek V.: *Simulační programovací systém Sipro.* Knižnice odborných a vědeckých spisů Vysokého učení technického v Brně, vol. B-41 Brno 1973.
10. Rudd D. R., Watson C. C.: *Strategy of Process Engineering.* Wiley, New York 1968.
11. Dohnal M., Jícha J., Klemeš J., Vašek V.: *Symposium on Use of Computer in Chemical Engineering*, May 15.—18., Ústí nad Labem, 1972.
12. Vermouzek Č., Vašek V., Klemeš J.: Chem. průmysl, *22*, 11 (1972).

Translated by V. Staněk.