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EXECUTIVE PROGRAMS FOR THE ANALYSIS AND STEADY STATE SIMULATION OF CHEMICAL PROCESSES

by

Yudh V. S. Jain

A DISSERTATION

Presented to the Faculty of

The Graduate College in the University of Nebraska

In Partial Fulfillment of Requirements

For the Degree Of Doctor of Philosophy

Department of Chemical Engineering

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Under the Supervision of Professor James M. Eakman

Lincoln, Nebraska

May, 1974

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TITLE

Executive Programs for the Analysis and Steady State Simulation of Chemical Processes

BY

Yudh V. S. Jain

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Y. V. S. Jain

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EXECUTIVE PROGRAMS FOR THE ANALYSIS AND STEADY STATE SIMULATION OF CHEMICAL PROCESSES

Yudh V. S. Jain

University of Nebraska, 1974

Advisor: Professor James M. Eakman

In this work, the problems associated with the generalized approach to the steady state simulation of chemical processes have been studied.

The structure of a chemical process, derived from its units and their connecting streams, is analyzed to determine the recycle nets and the sequential order of computation of units and recycle nets in the chemical process. This analyis is done by an 'identification program' based upon a compact matrix storage scheme and an efficient method for multiplication of matrices in compact form. Savings in both storage and computation time are achieved in this program.

An individual unit in the process is solved by a corresponding 'unit computation routine'. The simultaneous solution of all units involved in a recycle net is obtained by a convergence procedure which iterates on variables associated with a few selected streams, called cut streams. A 'heuristic tearing procedure' has been developed for the selection of an optimal cut set with minimum sum of

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weighting factors of streams. The proposed method gives better results than other heuristic methods for tearing.

A convergence method is formulated for the solution of recycle nets based on the concept of maximum use of available information in convergence promotion. The Jacobian needed in the convergence procedure is estimated from the results of initial iterations during convergence acceleration. The additional iterations required to compute a Jacobian by numerical differencing technique are thus eliminated in the suggested method.

The above mentioned programs have been incorporated into a system of executive routines for the steady state process simulation. The core storage requirements for the program are reduced by maintaining required data on external storage devices. The overall coordination, and data transfer operations in the simulation run are managed by executive routines. Some variables associated with cut streams may remain constant during convergence method in the solution of recycle nets. Such variables are removed from the basis of simultaneous equations. Thus the size of the set of equations is reduced. The restart option provided in the system, allows a simulation run to begin from the last point in a previous run.. The pertinent information required for resumption of a simulation run is stored on an external file.

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TABLE OF CONTENTS

PREVIEW

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LIST OF FIGURES

PREVIEW

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I. INTRODUCTION

Digital computers have been used extensively to solve chemical engineering problems since the beginning of their general availability. Their high speed and numerical accuracy have been effectively utilized to perform tedious and repetitive calculations which would have required large amounts of time if done manually. Methods which were considered infeasible because of the extensive computation involved, have been made possible through the use of computers. In addition to speed and accuracy, the modern computers have the capability to handle large amounts of information. New concepts in chemical engineering calculations, utilizing the latest innovations in computer hardware and software technology, are continuously being introduced. In particular, '<u>computer-aided process design</u>' and '<u>digital process control</u>' are but two new areas of research which have recently received considerable attention. The present work is concerned with computer-aided chemical process design.

The chemical process design, like most design activities, consists of two steps; '<u>process synthesis</u>' and '<u>process analysis</u>'. A final design is obtained by alternate application of these two steps. In process synthesis, a process designer outlines a processing scheme based upon physical and chemical laws, experience, intuition, and

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adopted conventions. A process scheme usually consists of selected pieces of equipment arranged in an appropriate order, so as to achieve desired changes in given raw materials. The process analysis involves an evaluation of a suggested processing scheme to determine its feasibility relative to the desired objective of carrying out the required process in a safe and economical manner. The results of a process analysis may suggest changes in the proposed scheme or they may indicate the necessity of an entirely new scheme. Alternate application of these two steps yields a design which may be accepted as final when the cost of carrying out an additional iteration becomes comparable to possible savings due to further improvements in the process.

Siirola et al. (1971) and Siirola and Rudd (1971) have reported the results of some recent research in the area of computer-aided process synthesis. However, it appears that much additional work will be required before the logical steps involved in a process synthesis are fully understood. A few heuristic methods for the synthesis of heat exchange networks (Lee et al., 1970), separation schemes (Thompson and King, 1972), and chemical reaction paths (Powers and Jones, 1973) have been proposed. Future work in this field should be of great interest to process designers and other chemical engineers alike.

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Both the dynamic and the steady state responses of a proposed processing scheme are required for a complete analysis of its performance. The dynamic behaviour of a process is needed to determine its stability and control characteristics. Material and energy flows in a process are provided by its steady state response. The evaluation of a process may be done either by pilot plant experimentation or by process simulation. The cost of extensive pilot plant experimentation is usually prohibitive and in recent times this method has become used increasingly for special cases only. In process simulation, the mathematical model for a processing scheme is developed from the knowledge of operations involved in it provided they are either well established theoretically or can be correlated empirically. This mathematical model is used to compute the unknown variables, representing the performance of the process, from the known variables in a specified processing scheme.

During the course of a process design, a number of processing schemes may need to be evaluated. Many of these processing schemes differ from one another only slightly. Writing a separate computer program corresponding to the mathematical model for each processing scheme, would require much repetitive, unuseful work. A general purpose program, which can simulate any specified process without requiring extensive programming, eliminates much of criticism. General programs are possible for both the dynamic

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simulation and the steady state simulation of chemical processes, but approaches to these two differ too widely to be considered together. This work is related to the development of a general purpose program for the steady state simulation of chemical processes.

A generalized steady state process simulation program is based on the concept of building blocks. Building blocks in this case are unit computational routines which perform the usual unit operation calculations in order to solve the states[1] of output streams from a specification of equipment configuration and operating parameters and the states of the input streams. Almost all units in conventional chemical processes can be simulated by presently available unit routines. In unconventional cases, routines for special types of units need to be written. Several programs for steady state simulation of chemical processes have been reported in literature. Evans et al. (1968) have reviewed some of these programs. A more recent survey on the state-of-art of such programs has been provided by Flower and Whitehead (1973).

In addition to solving each unit individually, a general purpose program should perform a series of other

---

[1]The "state" of a stream is defined as a vector containing information on the total mass flow rate, overall composition, enthalpy, temperature, and pressure associated with a stream.

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functions necessary to provide a complete analysis of the chemical process. These functions are summarized below:

1. Input of process specifications to the program.
2. Determination of recycle nets in process flowsheet.
3. Ordering of unit computations.
4. Selection of iterative variables in recycle nets.
5. Convergence of solution to recycle nets.
6. Data management between various routines of the program.
7. Control of overall simulation

These above mentioned operations in the simulation program are handled by a set of executive routines, built within the program package. In this dissertation, work has been done on the development of logical and mathematical methods, and corresponding executive routines for the analysis and steady state simulation of chemical processes.

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II. IDENTIFICATION

Digital computer simulation of chemical processes requires, in addition to the performance simulation of individual units, an efficient sequence of computation. This sequence depends upon the information flow within the process flow network. A unit can be simulated if the unit parameters and the input stream states are known. While unit parameters are usually specified, the unit input stream states may be the outputs of other units which must be simulated before the one under consideration can be treated. Some units can be easily arranged in a sequence. However, other units involved in recycle cannot be simulated individually because their inputs are dependent on each other. A set of units involved in a single recycle net is treated as a block in the computation sequence. Identification of a process flow network involves determination of the computation sequence of units and blocks (recycle nets), and finding the order of units and streams in every cycle of the block.

Two general approaches to the identification problem have appeared in the literature. Norman (1965) and Himmelblau (1966, 1967) have used matrix techniques for identification. Here a process flow diagram is considered to be a 'directed graph' (see e.g. Harary et al., 1965) and is represented by the corresponding adjacency matrix. Paths

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involving various numbers of units are determined from the corresponding powers of this adjacency matrix. The existence of cycles is shown by the presence of paths that start and terminate at the same unit. In Norman's approach the cycles are treated as they are found and the units involved are condensed into pseudounits. Maximal nets are determined when no more cycles exist in the condensed network. Himmelblau also uses the matrix method to determine the paths between units. The '<u>reachability matrix</u>' is defined by the Boolean summation of the subsequent powers of the adjacency matrix until a constant matrix results. Maximal nets are determined by consideration of mutually reachable units.

Steward (1965), Sargent and Westerberg (1964), and Christensen and Rudd (1969) have used the path-tracing techniques for identification. The process flow network is analyzed by considering the flow from one unit to the subsequent units. In this approach some of the units not involved in any recycle net are easily eliminated, whereas in the matrix approach all such units remain in until the completion of last calculations. Also, savings in the storage and computational time are usually obtained in the path-tracing methods compared to the matrix approaches. The practical advantages of the path-tracing methods seem to outweigh the notational advantage of the matrix methods.

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The method presented here is based upon a combination of both approaches. Improvements in the matrix related techniques have been made through the use of a compact storage for sparse matrices (adjacency matrices have in general only a small number of nonzero elements). Use of the proposed compact storage eliminates to a great extent some of the criticisms of the matrix approach. Multiplication of the matrices in the compact form by the proposed techniques results in a reduction in the computational time since unnecessary multiplication by zero elements is avoided. A path-tracing technique is employed only for the set of units in a single maximal net, thus reducing the size of combinatorial problem inherent in path-tracing techniques. The preceding and ending units are ordered prior to the determination of the cycles. The proposed method is formed by a combination of the following steps:

1. Formation of the adjacency matrix and its storage in the compact form.
2. Determination of maximal nets.
   - (i) location of cycles
   - (ii) separation of cycles
   - (iii) condensation of cycles
3. Ordering of units and blocks.
4. Determination of subcycles in a maximal net.

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ADJACENCY MATRIX AND ITS STORAGE

An adjacency matrix (see Figure 2.1) is formed from information concerning the streams of the process flow network. An element a_{ij} of the adjacency matrix represents the number of streams flowing from unit i to unit j. Most of the elements in this matrix are expected to be zero as only a few units receive the incoming streams from any specific unit. This spurious storage may be 10 to 15 times more than the actual storage required for nonzero elements. A reduction in storage is possible through the use of compact storage for the sparse matrices. Development of this technique involved consideration of the following points characteristic of most chemical process flowsheets:

1. Only a small number of streams originate from a unit as compared to the total number of units involved. (However no restriction has been placed on the total number of streams from a unit.)
2. The parallel streams if any are relatively few, thus listing them separately will not require excessive storage.

The adjacency matrix is stored as two vectors, the stream vector and the identification vector. The length of the stream vector is equal to the total number of streams in

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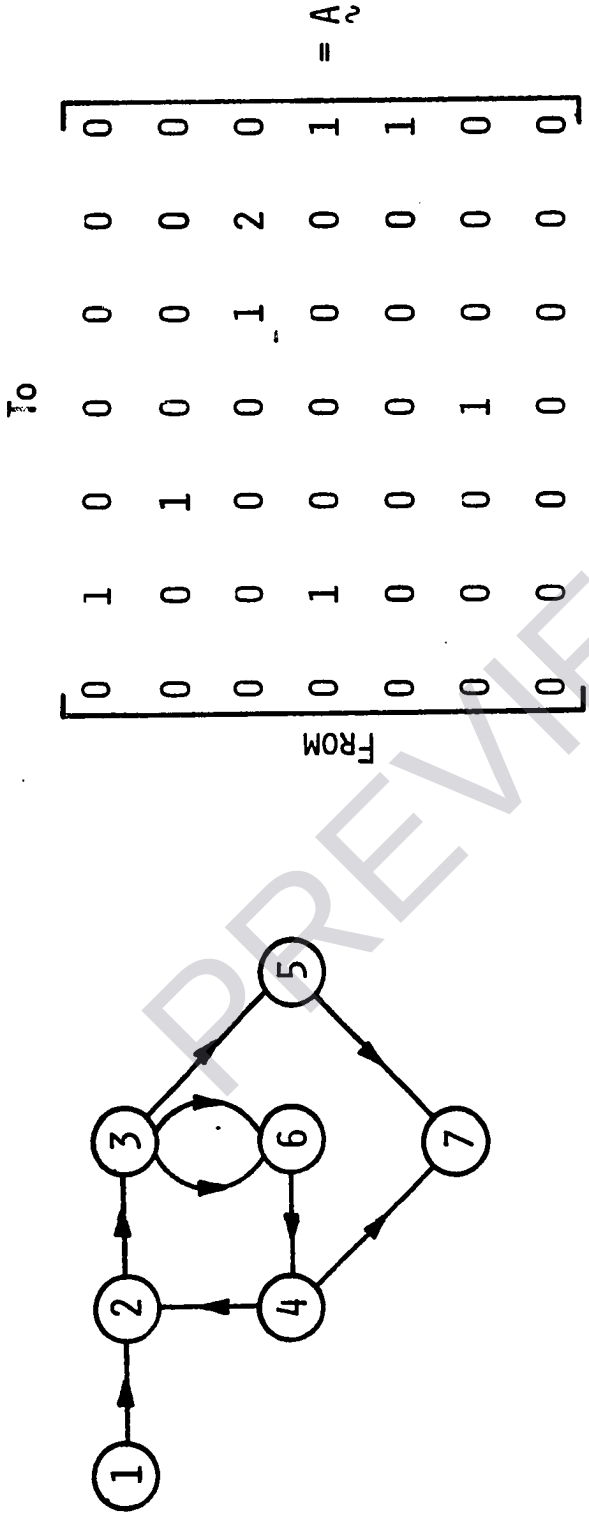

FIGURE 2.1 - A DIRECTED GRAPH AND ITS ADJACENCY MATRIX

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the network. The length of the identification vector is equal to the number of units.

Beginning with the unit designated number 1 in the process flow structure, the numbers corresponding to the units which receive flow from the first unit are listed in the stream vector in ascending order. In the case of n parallel streams the receiving unit is listed n times in succession. When all the streams which originate from the first unit have been listed, the index for the final position filled in the stream vector up to that point is stored in the first element of the identification vector. This procedure is repeated for streams originating from the second, third, etc.... units where numbers corresponding to the units receiving each stream are catenated to those already present in the stream vector. In each case the index of the stream vector position corresponding to the last stream originating from unit i is stored in the i-th position of the identification vector. The number of storage positions required by this technique is equal to the sum of the number of streams and the number of units in the process flowsheet. An 80 to 95% savings is typically realized in this approach as compared to the conventional technique in which the number of storage positions required is equal to the square of the number of units.

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The method can be illustrated by the example shown in Figures 2.1 and 2.2. There is flow from unit 1 to unit 2, so the number 2 is stored as the first element of the stream vector. There are no more streams from unit 1, so the first element of the identification vector is given a value 1. There is flow from unit 2 to unit 3, so the number 3 is stored as the next element of the stream vector. The second element of identification vector is assigned a value 2, since no more streams originate from unit 2. From unit 3, there is flow to unit 5 and two parallel streams to unit 6. Thus the next three elements of the stream vector are given the values 5, 6, and 6. This procedure is continued for streams originating from units 4, 5, and 6. In the case of unit 7, there is no outflow, thus no element of the stream vector is filled. The value of the seventh element in the identification vector is then the same as that of the sixth element, that is 9.

PREVIEW

This technique may also be expanded to allow other information about streams, such as stream numbers, weighting factors, etc...., to be stored within the same indexing framework as the entries in the stream vector.

DETERMINATION OF MAXIMAL NETWORKS

Many process flow networks contain units which are mutually reachable through a set of independent cycles. A

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$$\underset{\sim}{A} = \begin{array}{c} \\ \text{From} \end{array} \begin{array}{c} \text{To} \\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

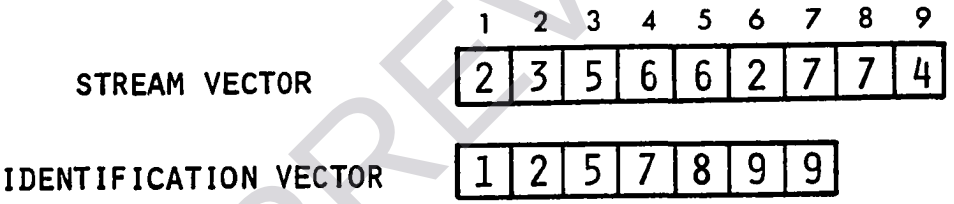

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FIGURE 2.2 - ADJACENCY MATRIX AND ITS COMPACT FORM

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