AN EVALUATION OF CONVERGENCE ACCELERATION

METHODS FOR CHEMICAL PROCESS

RECYCLE CALCULATIONS

By

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Submitted to the Faculty of the Graduate College
of the Oklahoma State University
in partial fulfillment of the requirements
for the Degree of
DOCTOR OF PHILOSOPHY
July, 1972

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PREFACE

This dissertation is concerned with providing an improved means of recycle convergence in block-type chemical process simulation. Several acceleration algorithms are tested on fourteen process problems. The problems represent industrial application, academic comparisons, and extreme test cases. Various modes of interaction are described with reference to the problems. None of the literature models are suitable for all these problems. Consequently, a modification of the Bounded Wegstein method is proposed, tested, and found to be superior to the other techniques. The result of using the new method is a general reduction in computer time and process iterations at a modest investment of computer core storage.

I would like to express my appreciation to Dr. John H. Erbar for his continual enthusiasm and encouragement given during the preparation of this thesis, and to the members of my committee, Dr. K. J. Bell, Dr. B. L. Crynes, and Dr. D. L. Fisher, for their suggestions and help. I appreciate the financial support which has been furnished by the National Aeronautics and Space Administration, the University Computer Center, and the School of Chemical Engineering with teaching assistantships. Also, I owe a great deal to my parents for giving me the opportunity to advance myself through education. Finally, I am grateful to my wife, Donna, who had no small share in the completion of this thesis.

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NOMENCLATURE

A   exponential factor for decay model

$^{\circ}$API   API gravity

b   molar component flow rate of a component in the bottom

         stream from a distillation column

C   criterion parameter

d   molar component flow rate of a component in the distillate

         stream from a distillation column

E_A desired fraction absorption

f(X)   individual component function of molar flow rate

$\overline{f}(\overline{X})$ calculated from stream vector $\overline{X}$

$\left|\dfrac{\partial f(\overline{X})}{\partial \overline{X}}\right|$ Jacobian of stream vectors

F   fresh feed for split fraction technique; also feed to process

         module

HK   heavy key component

i   the ith component

I   identity matrix (k x k)

K   equilibrium constant

k   the number of components in the system

L   total molar liquid flow

LK   light key component

n   the iteration number

NBPT   normal boiling point, $^{\circ}$F

$|P|$ process matrix for split fraction method

$|q|$ linear parameter matrix for forcing method

q_i the linear Wegstein parameter for component i

V total vapor flow

X individual componential molar flow rate

$\overline{X}$ stream vector; also total feed vector for split fraction technique

$\overline{X}_o$ initial guess for stream vector

z Orbach and Crowe damping factor

z_{jm} fraction of feed to jth module to product m of the module

$\overline{\alpha}$ true solution vector

γ_n error vector between calculated and true solution

Δ tolerance value

λ Orbach and Crowe application parameter

LIST OF SYMBOLS
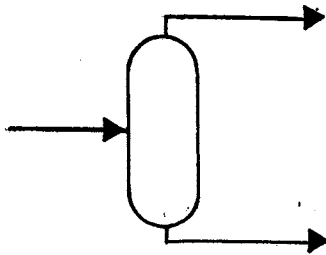
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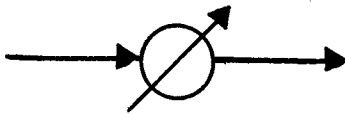
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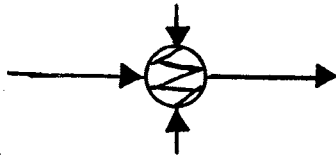
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Input or Output Blocks
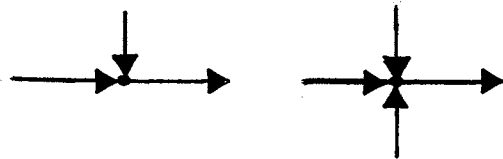
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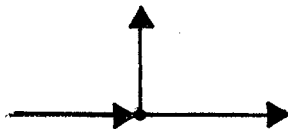
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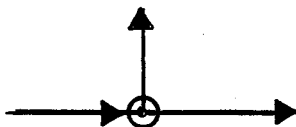
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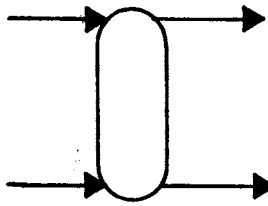
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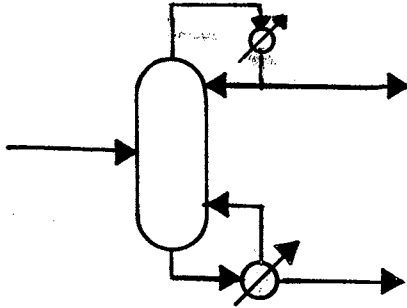
Distillation Column

Compressor or Expander
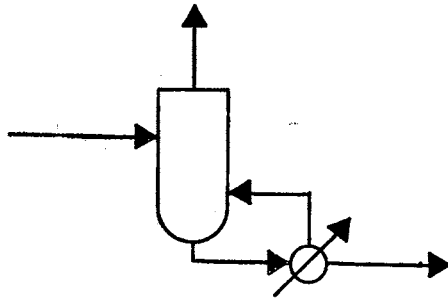
Stabilizer Column

Pump

Reactor

CHAPTER I

INTRODUCTION

The advances in computer technology, larger core memories and faster operation times, have led to the development of large, highly sophisticated chemical process simulation systems. These systems are used to calculate the performance of a variety of chemical processes. More alternatives can be evaluated by the process engineer due to these advancements. In addition, more complex methods may be applied to the evaluation of the performance of process equipment. In general, process flow systems fall into two broad categories: acyclic and cyclic systems. The flow diagrams of typical flow systems are shown in Figure 1. Acyclic systems may be analyzed from only one evaluation of each processing unit. Cyclic (recycle) processes, however, involves the return of material and/or energy from a later point in the system to an earlier point. Since the recycled stream may result in a change in the feed rate, composition, temperature, or phase split to the modules that have been previously calculated, the solution requires a reevaluation (iteration) of the process system.

The typical form of the iterative solution is given by Equation (1).

$$\overline{X}_{n+1} = \overline{f}(\overline{X}_n) \qquad (1)$$

1

Such a form is a common iterative solution in many branches of mathematics. Two important features are different. First, the quantity $\overline{X}$ represents a stream vector that may represent as many as sixteen or more molecular species. Not only is the problem multidimensional, but also each of the molecular species interacts one with another. Such quantities as the equilibrium constant are a function of the composition of the fluid stream. Secondly, the stream function f is a conglomerate of many functions due to the configuration of the process flow. To complicate the case further the behavior of most process elements is highly nonlinear. The functions, which are used to represent the process elements, usually are not explicit, but instead are of an iterative nature. This iterative nature is due to the nonlinear physical properties associated with each molecular species. For example, consider the simple adiabatic flash system presented in Figure 2. The basic operation of such vapor-liquid separation elements is represented by Equation (2).

$$0 = \sum_{i=1}^{k} \frac{(1+L/V)(F_i/F)}{1+L/(K_i V)} - 1 \tag{2}$$

The basic variables are composition, temperature, and pressure. The equilibrium constant is typically a function of temperature and pressure as shown in Figure 3. Thus the nonlinear function becomes iterative whether one is seeking the temperature, the pressure, or the feed split to the vapor and liquid. After the split is determined the material balance is complete, but the respective streams must undergo the heat balance procedure. Enthalpy as a function of temperature and pressure typically may be represented in Figure 4. Here again another

nonlinear function is applied to the process stream. The nonexplicity, nonlinear nature of the simulation of a flash element is now apparent. The operation of the flash element is now apparent. The operation of the flash element is typical of many of the other elements. Rigorous analysis of absorber and distillation units require simultaneous solution of some number of interconnected flashes and many require as many iterative computations as the number of equilibrium stages in the units. Thus the process function f is a complex, nonexplicit function that is not susceptible to mathematical analysis per se.
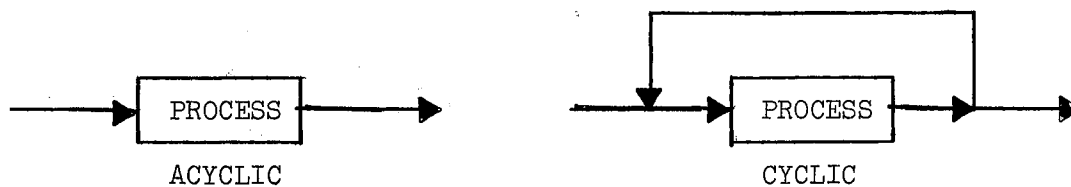
Figure 1. Types of Flow Patterns
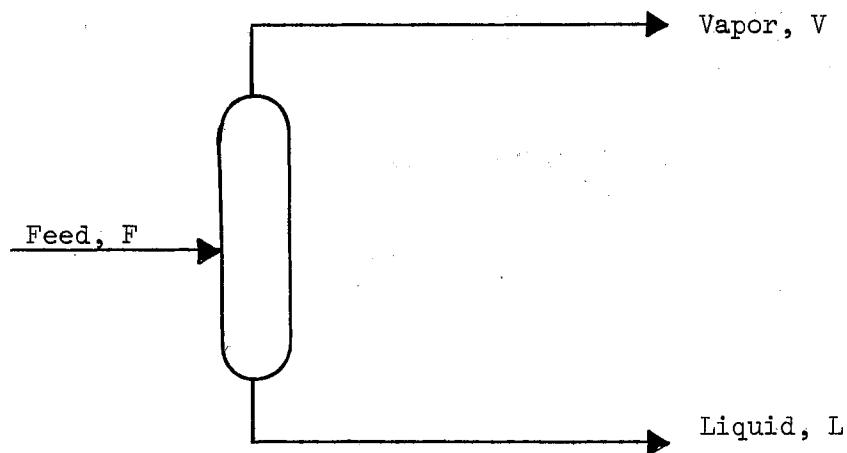
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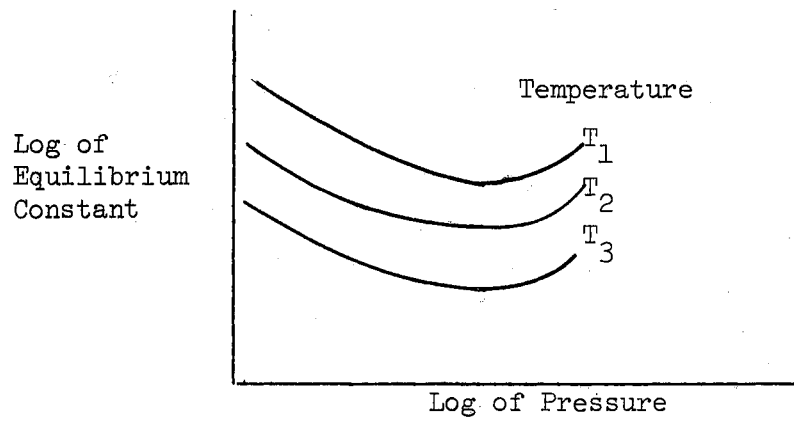
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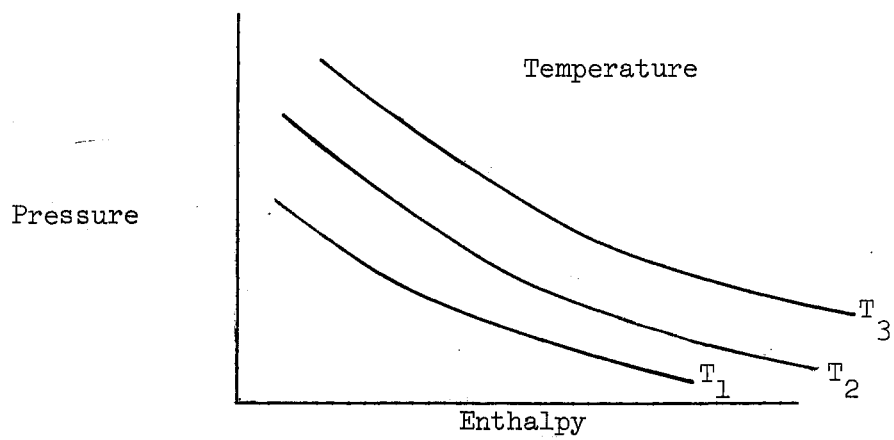
Figure 4. Enthalpy of a Typical Component

This work is concerned with the number of iterations needed to obtain the final answer in overall heat and material balances (process evaluations). The problem of internal simulation of the modules is not considered.

Many techniques (recycle convergence accelerator algorithms) have been advocated in the literature to decrease the number of process evaluations. The ultimate goal of such algorithms is to lessen the cost of simulation and permit more process evaluations to be made. Usually, the reports of such procedures have been in theoretical terms and not accompanied by illustrations of actual industrial applications. The objectives of this work are, therefore, to explore the literature for possible acceleration procedures, to test the promising algorithms for possible applications, and to provide a more general evaluation of the procedures based on iterations, time, and core storage. Fourteen problems are selected for this study in three areas. The areas are: (1) available problems with direct industrial application, (2) academic problems found in the literature for purposes of comparison, and (3) synthetic problems formulated to illustrate an extreme example. Erbar (2) has developed a steady state process simulator. The simulation, called OSUPAS, permits the use of a variable flow sheet. Implementing some of the algorithms in OSUPAS and applying the simulation to some realistic industrial processes, the acceleration patterns are examined and compared. Finally, by means of suitable determined comparisons, a recycle convergence acceleration procedure is developed for the OSUPAS simulator.

CHAPTER II

LITERATURE SURVEY

In order to understand the problem of recycle convergence
acceleration, an appreciation of both simulation systems and the
acceleration algorithms must be gained. The simulation systems have a
complex organization to deal with the sequential calculation of many
flow configurations. Since the iterative simulation problems are
imposed upon the user, many attempts have been made to improve the
recycle convergence. Simulation systems and acceleration algorithms
are the subjects of interest for the establishment of background
experience in the field of recycle convergence acceleration.

Characteristics of Simulation Systems

The purpose of the generalized block type simulation design tool
is to provide a means of evaluating a number of design alternatives
such as:

1. Allowing a variable flowsheet.

2. Using evaluation techniques commensurate with the accuracy
   required.

3. Handling a given problem with physical properties and other
   unspecified data in a self-contained format.

4. Providing an effective interface between the system and the
   user in the input and output phases.

The key to successful usage of a generalized system is the flexibility
of the system. If a large number of process modules are available to
the user, more flowsheets may be processed and fewer hand evaluations
or special computer programs are necessary. Along with the presence of
a number of available modules, the option to perform the simulation at
various levels of rigor should be available to the user. For a pre-
liminary evaluation, where design parameters are uncertain, shortcut
techniques would be satisfactory. When the final design determinations
are being made, more rigorous techniques would be in order.

A convenient physical and thermodynamic property prediction package
must be available for each component in the total stream vector. Such
factors as enthalpy, phase split, and density must be derived from
temperature, pressure, and composition information. OSUPAS uses a
standard thermodynamics property prediction method, (2). Non-discrete
(or non-standard) components, such as an absorber oil fraction, called
hypothetical components, may be characterized by means of API gravity,
average molecular weight, and normal boiling point. The input sequence
of the simulation system determines the amount of effort required to
learn how to use the tool. A simple language and clearly defined input
format can put the design tool in the hands of a well-informed non-
technical person. Some simulation systems provide so many options with
such detailed input data required that considerable technical evalua-
tion must be conducted before they can be used. Similarly, the output
phase determines who can evaluate the results.

The many different block-type design systems have certain features
in common. The process flowsheet and process data pertaining to the
individual modules must be defined in the input phase. Control

information such as tolerance levels and iteration limits for recycle processes must be defined. This information is then transferred to an executive subroutine which is responsible for the operation of the over-all simulation. The executive subroutine must digest the input information, generate a process matrix defining the sequence of calculation and the route of the numbered streams, assimilate the design data parameters for each module and provide in the detail data parameters for each module as provided in the input data, carry out the calculations in some designated sequence, and produce answers with sufficient detail for analysis.

The solution to the given problem as presented to the executive subroutine proceeds in three phases. The first phase involves checking the input for correct format and completeness. If the presented data are not correct, further analysis would be pointless and the run is aborted. Additional checks are made on the operating range of the data. The second phase involves the sequential evaluation of the described unit operations. When the calculations are complete, the feed to any module will not have changed by more than a specified amount from the previous iteration. When an iteration is finished and the recycle streams, if any, have been converged, then the output phase is begun. Here adequate data are presented for the evaluation of the process including the stream-by-stream heat and material balances.

Because of the demand for computer simulation of chemical processes, a number of generalized simulation systems have developed. CHIPS, FLOWTRAN, PACER, FLOWSCRIPT, GENDER, and OSUPAS are among the many simulations that have been devised, Sargent (16). All share the

basic concepts, needs, and problems of generalized process simulation, namely:

1. Modularity, that is the independence of process modules.

2. The ability to perform the appropriate process calculations in some designated sequence.

3. Effective and appropriate communications between the user and the computer.

Many specific problems are encountered during simulation. Each system must be prepared for contingencies such as an iterative procedure to handle recycle streams. Furthermore, it is important to recognize that such simulation programs are a good deal more than just conglomerates of unit operations.

Recycle Convergence Acceleration Algorithms

Since the advent of the computer simulated process solution, workers have been searching for means to shortcut the tedious iterative schedule of cyclic calculations. The forms of the acceleration algorithms employed over the twenty year history of such investigations have run the gamut of mathematical sophistication ranging from intractable algorithms with many partial differentials to coarse curve fitting. In each case, it is advantageous to know the answer or at least the pattern of convergence prior to attempting the solution. In the following pages a brief synopsis is presented of some of the more widely known convergence methods and their relationships to one another. In the current literature, the methods most frequently considered are:

1. Geometric fitting.

2. Successive substitutions with forcing.

3. Newton-Raphson.

4. Wegstein and Pourciau.

5. Dominant eigenvalue.

6. Split fraction.

These methods are applicable to generalized process simulation where optimization procedures cannot be used due to the lack of explicit equations for various modules.

Successive Substitutions

The simplest procedure from a programming stand-point is successive substitutions. Successive substitutions, as the name implies, involves the solution of a previous trial being used to calculate the answer of the next. For a sample process, the relation between $\overline{X}_n$ and $\overline{X}_{n+1}$ for recycle stream vector $\overline{X}$ is illustrated in Figure 5. Since n and n+1 correspond to successive iterations, the solution $\overline{X}_{n+1}$ will replace $\overline{X}_n$ on the $(n+2)^{th}$ iteration. The stream vector is repeatedly reestimated until $\left|\left|\frac{(X_{n+1} - X_n)}{X_n}\right|\right|$ maximum componential flow rate $\leq \Delta$ where Δ is a specific tolerance. Only two factors need to be noted here:

1. $\overline{X}_o$, the initial guess for the recycle stream vector, may either be assumed to be zero (some processes will not converge with this assumption) or some finite value set at the user's discretion.

2. Δ may take more than one form. Some methods define Δ as previously stated. Others select $\Delta < \sum_{i=1}^{k} \frac{(X_{n+1} - X_n)^2_i}{X^2_{i,n}}$ where k is the number of components. For this reason some confusion about the convergence tolerance has arisen.
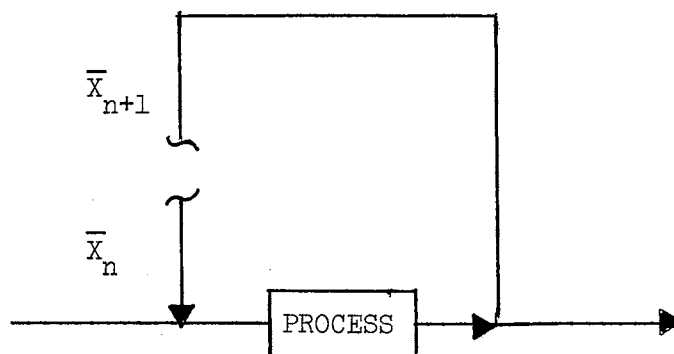
Figure 5. Typical Recycle Scheme

Geometric Algorithms

The simplest type of acceleration algorithm fits a geometric form
to a convergence pattern. The convergence schemes for the chemical pro-
cesses converged by successive substitutions appear to be exponential
in form as shown in Figure 6. Such a function to determine the solution
vector, X, is proposed by Isakson (3) and presented in Equation (3).

$$X_i = \alpha_i (1 - e^{An})$$

Although the total stream flow rate appears to follow this general
functional form, the individual component flow rates do not neces-
sarily converge monotonically or fit the specified form even if
monotonically increasing. Poor convergence characteristics may be
associated with the lack of independence of the components.
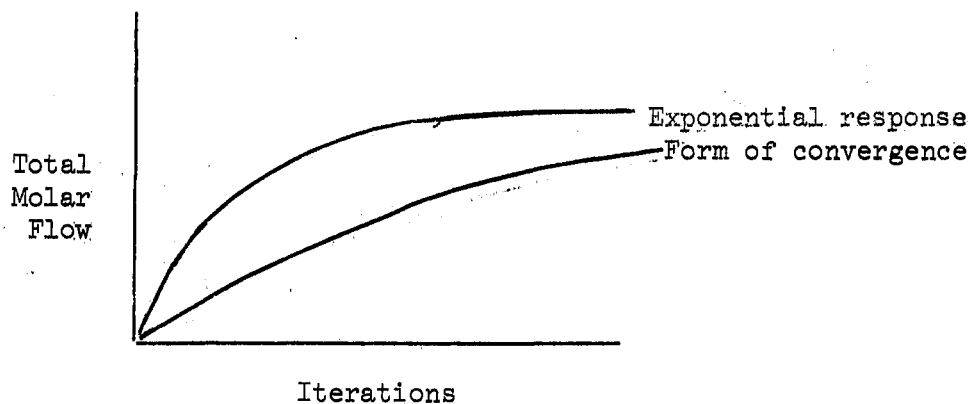
Figure 6. Typical Response Patterns

Since independence between variables may be characterized by the partial derivative of componential flow rates, convention places all the combinations of the partial derivatives in a matrix called a Jacobian. Further, because of the nature of the stream vector, molar flow rates are considered the Jacobian variables in this instance (the form is $\overline{X}_{n+1} = \overline{f}(\overline{X}_n)$) as shown in Equation (4).

$$\left| \frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}} \right| = \begin{bmatrix} \frac{\partial f_1}{\partial X_1} & \frac{\partial f_1}{\partial X_2} & \cdots & \frac{\partial f_1}{\partial X_k} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_k}{\partial X_1} & \frac{\partial f_k}{\partial X_2} & \cdots & \frac{\partial f_k}{\partial X_k} \end{bmatrix} \qquad (4)$$

If the condition of independence is satisfied, all partial derivatives off the main diagonal are zero.

Since two parameters (α and A) are involved in Isakson's algorithm, the first accelerated point cannot occur until the process has been evaluated twice. Once the parameters are calculated the acceleration step may be applied to each successive iteration. Isakson fails to apply the procedure to any chemical process system. Apparently the intended use of the method is in mechanical systems work. Another version of the same approach, presented by Cavett (1). The form of the model function is a rectangular hyperbola. After basic algebra, the algorithm takes the form given by Equation (5).

$$X_{2n+2} = X_{2n+1} + (X_{2n}-X_{2n+1}) \left[1-\frac{(X_{2n-1} - X_{2n})(X_{2n}-X_{2n+1})}{(X_{2n-1}-X_{2n})(X_{2n}-X_{2n+1})-1} \right] \qquad (5)$$

The procedure may be used after the second iteration and then repeated on alternating iterations. The algorithm suffers from the same problems as does the exponential form. The variables must be independent and the form of the convergence pattern must be reasonably close to a rectangular hyperbola. Cavett tests the hyperbolic algorithm on typical gas-liquid separation systems, Figure 7, and obtains a net reduction of six iterations. Cavett, however, does not report the results of the procedure on a flash network, Figure 8. Further, the convergence is not monotonic, but rather has the appearance of a saw-tooth which indicates that the assumption of independence is not completely valid.

Successive Substitutions With Forcing

Kliesch (4) developes several algorithms in his dissertation. Among the algorithms discussed are successive substitutions with

forcing and Newton's method. To aid in understanding Newton's and the forcing methods, a criterion for convergence for successive substitutions is first derived.

The general pattern of the convergence scheme for successive substitutions proceeds as follows (where f is the process function internal to the recycle loop considered) in Equation (6).

$$\overline{X}_{n+1} = \overline{f}(\overline{X}_n) \tag{6}$$

Again, the main difficulty with this expression is that f is not usually explicit, so that the derivatives cannot be analytically determined. This expression is useful in deriving a convergence criterion and as a springboard to the development of some acceleration methods.

The representation of $\overline{X}_n$ as the sum of $\overline{\alpha}$ (the true solution) and $\overline{\gamma}_n$ (the error of the nth iteration) may be made. By means of a first order Taylor's series expansion about the true solution $\overline{\alpha}$, Equation (6) becomes Equation (7).

$$\overline{\gamma}_{n+1} + \overline{\alpha} = \overline{f}(\overline{\alpha}) + \left| \frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}} \right|_{\overline{X}=\overline{\alpha}} \overline{\gamma}_n \tag{7}$$

Since a first order approximation implies linearity, the slope is constant and may be evaluated at any point on the function. The partial differential of the vector takes the form of a Jacobian as is presented in Equation (4). The nature of process convergence implies that at the solution all slopes go to zero. But obviously, if all slopes go to zero at the solution, the function cannot be linear, and the original assumption is defunct. Since nonanalytical second derivatives are difficult

to accurately determine, linearity is used as approximation. In any event, if the slope of the process function is zero at the solution, then this may be represented by Equation (8).

$$\bar{\alpha} = \bar{f}(\bar{\alpha}) \qquad (8)$$

The next step is to reduce Equation (7) by making the solution vector substitution as reduced in Equation (9).

$$\bar{\gamma}_{n+1} = \left| \frac{\partial \bar{f}(\bar{X})}{\partial \bar{X}} \right| \bar{\gamma}_n \qquad (9)$$

From the rules of matrix multiplication, the rule for convergence may be established in Equations (10, 11, and 12).

$$\text{If } \bar{\gamma}_{n+1} < \bar{\gamma}_n \text{ for all } n \qquad (10)$$

and

$$\sum_{j=1}^{k} \left| \frac{\partial f(X_i)}{\partial X_j} \gamma_{nj} \right| = \gamma_{(n-1)_i} \qquad (11)$$

convergence cannot be guaranteed unless Equation (12) is satisfied.

$$\sum_{j=1}^{k} \left\| \left| \frac{\partial f(X_i)}{\partial X_j} \right| - \right\| \ll 1 \text{ for all } i \qquad (12)$$

Since the slope is the greatest at the beginning of the successive substitutions procedure, the criterion may be evaluated after one iteration to determine if convergence is assured. This principle corresponds roughly to a multidimensional Lipschitz condition. Since typical behavior has shown that the slope usually is quite steep at

the beginning to the solution (see Figure 20), there is not much
likelihood of the condition being satisfied.

A linear combination of $\overline{X}_n$ and $\overline{f}(\overline{X}_n)$ is the basis for convergence
procedure with forcing. A linear combination of two iterative results
is formed in Equation (13), then Equations (14) and (15) solve for
the linear factor q.

$$\alpha = \left|q\right| \overline{f}(\overline{X}_n) + (\left|I\right| - \left|q\right|)\overline{X}_n \tag{13}$$

$$\left|\frac{\partial\overline{\alpha}}{\partial\overline{X}}\right| = \left|o\right| = \left|q\right| \left|\frac{\partial\overline{f}(\overline{X}_n)}{\partial\overline{X}}\right| + (\left|I\right| - \left|q\right|) \tag{14}$$

$$\left|q\right| = \left[I - \left|\frac{\partial\overline{f}(\overline{X}_n)}{\partial\overline{X}}\right|\right]^{-1} \tag{15}$$

An expression is obtained that would rigorously provide the solution
vector if the system were linear. The procedure contains the standard
difficulty that a number of convergence accelerators have, namely,
the determination of the derivatives by perturbation requires additional
iteration through the system. If the number of components is fifteen,
the fifteen perturbation iterations which are required increase the
iteration time fifteen fold.

Newton-Raphson Algorithm

For completeness, no convergence acceleration discussion is
thorough without the Newton-Raphson first order approximation. Start-
ing with a first order Taylor series representation of $\overline{f}$, Newton's
method is derived in Equations (16, 17, and 18).

$$\overline{f}(\overline{X}_n) = \overline{\alpha} + \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|(\overline{X}_n - \overline{\alpha}) \tag{16}$$

$$\overline{f}(\overline{X}_n) - \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|\overline{X}_n = \overline{\alpha} - \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|\overline{\alpha} \tag{17}$$

$$\left|I - \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|\right|^{-1}(\overline{f}(\overline{X}_n) - \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|\overline{X}_n) = \overline{\alpha} \tag{18}$$

This expression can be shown to be the same as the previous forcing method complete at the solution point with the same first order approximation and derivative calculational difficulties.

Of significance at this point is the redefinition of the process function to another function such that $\overline{h}(\overline{\alpha}) = \overline{f}(\overline{X}_n) - \overline{f}(\overline{\alpha}) = 0$. When this is applied to the Newton-Raphson solution system, Equation (19) assumes a more familiar form.

$$\overline{X}_n - \left|\frac{\partial \overline{f}(\overline{X})}{\partial \overline{X}}\right|^{-1}\overline{f}(\overline{X}_n) = \overline{\alpha} \tag{19}$$

Such redefinitions in process modules would be difficult. The form is presented here for comparison.

Obviously, a large number of pertubation iterations would damage the convergence acceleration with respect to time. Cavett (1) suggests the possibility of evaluating only the major components of the process stream. As yet the criterion for selection has not been successfully developed as is demonstrated in Cavett's work. Newton's method is applied by Cavett to both Problem 2 and 7, Figures 7 and 8. In Problem 7 the method converges in fifteen iterations compared with fifty-five iterations for successive substitutions. However, the time of solution is proportional to the number of process evaluations,
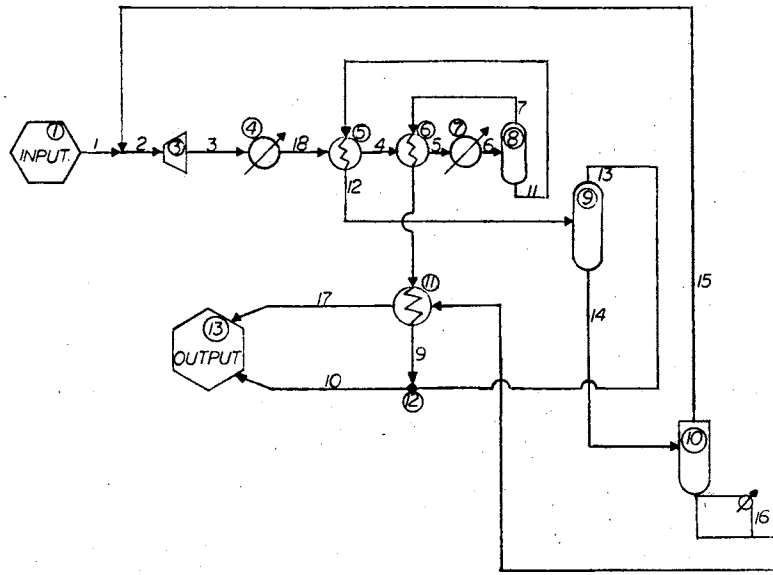
Figure 7. Cavett's Second Problem
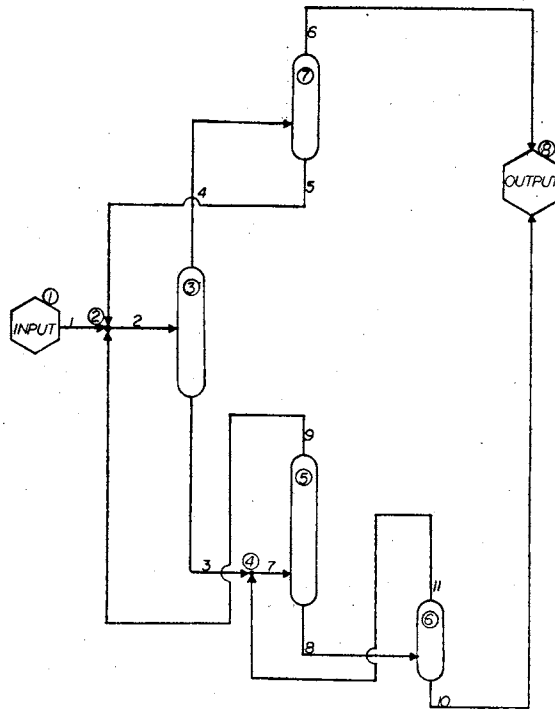
Figure 8. Cavett's First Problem

the time for the Newton's method solution is increased by a factor of

4.63 over the successive substitutions solution time as shown by

Equation (20).

$$\text{time ratio} = \frac{\text{solution time for algorithm}}{\text{solution time for successive substitutions}} =$$

$$\frac{(K+1)\ \text{Newton's}}{N_{s,s}} = \frac{(16 + 1)\ (15)}{55} = 4.63 \tag{20}$$

Attempts to use only some of the derivatives leads to even poorer

results. Newton's method applied to Problem 2 yields a time ratio of

7.32. The analysis here only considers time, but also additional

storage would be required to implement Newton's method. Kliesch also

evaluates Problem 7 by successive substitutions and Newton's method.

The results of the work yield a solution time ratio of 3.52. On the

whole, Newton's method leaves much to be desired in terms of the time

for solution. However, in the most sophisticated simulation systems,

analytical derivatives are becoming available. As the derivatives

of process modules become generally available, time factors become

more inviting for Newton's method as well as the iterative method with

forcing. Considering this evidence, a decision to forego any further

examination of Newton's method has been made for this work.

Wegstein Algorithm

The Wegstein method of iteration acceleration is also examined by

Cavett. Pourciau (14) proposes the concept of a solution being a

linear combination of any two iterations. Lacking a method for

evaluating the linear parameter, the parameter is simply assumed to be a constant or altered in a sequential method between two bounds. However, the value of the parameter must be empirically determined for the particular process system being evaluated. The difference between the Wegstein and successive substitutions method with forcing lies in the fact that each component is treated independently by Wegstein (17) thus avoiding the necessity of obtaining k partial derivatives and inverting the subsequent matrix. The expression for q_i (for the ith component) can be developed by modifying Equation (15) to Equations (21) and (22).

$$q_i = \frac{1}{(1 - \frac{\Delta X_{n,i}}{\Delta f_{n,i}})} \tag{21}$$

$$\alpha_i = q_i \, f_i \, (X_{n,i}) + (1-q_i) \, X_{n,i} \tag{22}$$

Clearly, the case for componential independence is not strong in many process circumstances. Wegstein (17) noted in the application of the algorithm that unless $\left\|q_i\right\|$ remains less than unity, the procedure would cause a divergence between the iteration solution and the true solution. Cavett has applied the procedure to Problem 2 and found an iteration reduction from twenty-one to twelve. Apparently, the independence assumption is not suited to Problem 7 since results for the method are not indicated.

Kleisch has noted Wegstein's criterion for divergence of the algorithm and reasoned that if the value of q_i is constrained not to exceed the bound of one, the procedure would be forced to converge.

Making this observation, the technique called the "Bounded Wegstein"
is applied to Problem 7 by Kleisch and a time ratio of 0.763 is
obtained. On an ammonia synthesis loop developed by Klesich the
Bounded Wegstein has given a time ratio of 0.583. Apparently, the two
cases that Kliesch tests lie in the gray region: too much interaction
for the technique to be rigorous, but not enough interaction for
detrimental oscillation in the method to occur.

Dominant Eigenvalue

Orbach and Crowe (12) have done the most recent available work in
the area of first order convergence accelerators. Essentially, the
method uses the eigenvalues of the Jacobian based on the molar flow
rates of the stream vector. From the value of the largest eigenvalue
that is associated with the Jacobian, the convergence may be tested and
a solution may be predicted. Through algebra, as shown in Equations
(23) through (28), the algorithm of Orbach and Crowe may be seen to be
identical, with one exception, to the Wegstein.

$$\bar{\alpha} = \bar{X}_{n-1} + \frac{Z(\bar{X}_n - \bar{X}_{n-1})}{(1-\lambda)} \tag{23}$$

$$\text{where } \lambda = \left|\Delta X_n\right| \Big/ \left|\Delta X_{n-1}\right| \text{ max componential flow rate} \tag{24}$$

$$\text{or } \lambda = f' \tag{25}$$

From the previous algorithms for the maximum component j,

$$1-q_j = \frac{1}{(1-\lambda_j)} \tag{26}$$

$$1 - \frac{1}{1-1/f_j'} = \frac{1}{1-f_j'} \qquad (27)$$

$$\frac{1}{1-f_j'} = \frac{1}{1-f_j'} \qquad (28)$$

There is only one value of λ for all the components of the system. The authors suggest that the method does not ignore the lack of independence between the variables, but at the same time does not deal with the problem explicitly. Disregarding the interaction problem is not a recommended method of obtaining the solution. Additionally the empirical criterion for the application of an acceleration step is that the value of λ on two successive iterations be less than 0.5%. Also the value 0.7 for the damping factor z is used. When the algorithm is applied to an alkylation plant, a time ratio of 0.40 is obtained. Orbach and Crowe also apply the "Wegstein" method and find "unstable oscillations."

Other Algorithms

Over the years, many other methods have been proposed along the lines of scaling toward the final answer based on previous iterations. Cavett tests one such method called relaxation. Relaxation involves a holding tank approach to a dynamic solution. When the tank input matches the output, the solution is said to occur. However, when applied to Problem 7, a time ratio of 4.40 is obtained.

Ravicz and Norman (11) use a nonlinear programming approach to calculate the results of the recycle network. The problems are solved by means of a Newton-Raphson approach. Since the Newton-Raphson

method requires iterations to evaluate the partial derivatives, Napthali (10) reduces the complexity of the problem by removing the dependent variables from consideration. The variable reduction is accomplished by means of nodal material balances. The values of the unspecified independent variables are then altered by the Newton-Raphson procedure. A Fibonacci search is then used to explore the region between the preceding value and the predicted value by use of an objective function. The objective function is the discrepancy in the overall material balance. Law and Fariss (5) extend this approach to an optimization problem. They present a method called rotational discrimination which corresponds to a nonlinear programming problem. The method is quite rigorous but is unsuitable for simulation procedures due to the complexity of surfaces generated in process simulation techniques and the cumbersome evolution of new vector values as confirmed by Kliesch. Other methods have been proposed but have no applications recorded in the literature and are included in the literature review presented by Kliesch.

Split Fraction Material Balance

Still another approach to the simulation problem has been formulated by Nagiev (9). A material balance expression is written for each component, characterizing each module by splitting a portion of the input into each product stream. Essentially, the process attempts to linearize the highly nonlinear operation of the process modules. The resulting balance then takes the form as shown by Equations (29) and (30).

For a single module and component,

(29)

Fresh Feed = Total Feed − Feed from Other Modules

For a process system and single component,

(30)

$$\overline{F} = \overline{X} - \left|P\right|\overline{X}.$$

The matrix $\left[P\right]$ is a function of the configuration of the process modules as well as linear splits. For example, one may wish to consider a process system as shown in Figure 9. The material balance equations for a single component i are Equations (31) and (32).

$$F_i = X_{1i} - z_{2a}X_{2i}$$ (31)

$$0 = X_{2i} - z_{1a}X_{1i}$$ (32)

The matrix notation for the equations is given by Equation (33).

$$\begin{bmatrix} F_i \\ 0 \end{bmatrix} = \begin{bmatrix} 1 - z_{2a} \\ -z_{1a} & 1 \end{bmatrix} \begin{bmatrix} X_{1i} \\ X_{2i} \end{bmatrix}$$ (33)

The result of a single process iteration is an incorrect material balance due to changes in modular operation (split fraction) resulting from feed modifications. The method of Nagiev proposes that the material balance be completed in one step as given by Equation (34) rearranging the matrix equation.

$$\begin{bmatrix} X_{1i} \\ X_{2i} \end{bmatrix} = \begin{bmatrix} 1-z_{2a} \\ -z_{1a} & 1 \end{bmatrix}^{-1} \begin{bmatrix} F_i \\ 0 \end{bmatrix}$$ (34)

The difficulty is obtaining the correct split fractions which Nagiev assumes to be constant over the course of the solution. The obvious flaw, which seems to be standard by now, is that all components are treated separately and independently.
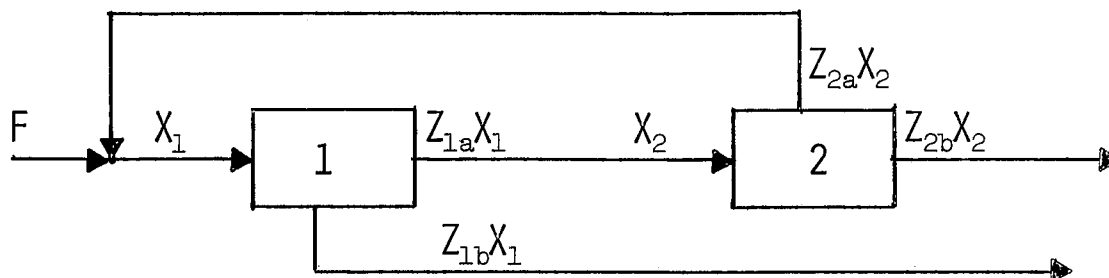
Figure 9. Sample Recycle Process for Split Fractions

Rosen (15) recognizes the variance of the split fractions and proposes to revise them by iteration. In this manner, the dependence of each variable is adjusted in each iteration even though the interdependence is not formally considered by the algorithm. Rosen also has developed a procedure which would cause components to appear and disappear due to chemical reactions. Kliesch does not consider Rosen's treatment of chemical reactors useful. Use of the split fraction method is generally restricted to process modules with only one feed. The specified $\overline{X}_j$ is the total feed to the jth module. Therefore, if the module has more feed, some supplementary material balance has to be used.

One of the advantages of the split fraction approach is that

split fractions are bounded between 0 and 1. These fractions are stable which permits more effective use of acceleration means. Rosen examines a simple reactor system by the split fraction formulation with a Pourciau acceleration algorithm (q = 0.5). Unfortunately, no comparison is made with successive substitutions, and no time ratio is available. Kliesch also tests the split fraction formulation on Problem 7. For the direct split fraction formulation and the split fraction technique supplemented with Pourciau acceleration (q = 0.2), time ratios of 0.944 and 0.916, respectively, are obtained. Strangely enough, Kliesch does not apply the Bounded Wegstein method to the split fractions in the algorithm. The apparent disadvantage to the split fraction procedure is the time required to invert the matrices. In addition the number of inversions are equal to the number of components in the system.

Other acceleration methods are known and compiled by Sargent (16) along with a great deal of information concerning the philosophy and organization of many simulation systems. Of course, many industrial simulation systems, which are proprietary, may have successfully dealt with the recycle convergence problem.

Optimization Techniques

A more recent approach to increasing the efficiency of computerized calculations are the optimization techniques. In 1963, Cavett, in applying recycle convergence accelerators, terms optimization techniques as "not very useful," referring to nonlinear programming solutions. Work reported recently by Rudd (6, 7, 8) extends the idea of optimal sequences of calculations and design variable selection for the modules without the benefit of nonlinear programming.

A paper by Lee, Christensen, and Rudd (6) sets forth criteria to select design variables. The analysis of the number of degrees of freedom in a given design problem specifies the selection of a number of variables called design or decision variables. The authors suggest that by judicious selection of these variables the magnitude of the design problem may be reduced. Through graphical methods, the inter-relationship of variables is studied. Algorithms are devised based upon these graphs to specify the proper number of design variables (corresponding to the degrees of freedom analysis) and a minimal modular interaction scheme. Examples to show the usefulness of the technique are devised and in some cases, cyclic problems are converted to acyclic problems. Unfortunately, in generalized simulation procedures such as OSUPAS, the explicit equations needed to make such evaluations are unavailable. Further, the specification of the decision variables for calculational purposes is such that simulations are, in general, not capable of such optimization.

Lee and Rudd (8) report a method for sequencing modular calcula-tions to reduce the number of recycle streams presented for calcula-tion. The objective of such an analysis is recycle stream tearing (breaking a recycle stream with the subsequent assignment of a value) to create an acyclic process. Since an additional objective is to minimize the number of tears, the order of calculation is altered. Through a sequence of matrix operations, algorithms are used to select the proper sequence of calculation. The obvious drawback is that the calculational sequence is fixed for process simulation by the known quantities such as feed rate. When a good estimate of the recycled quantities or selected modular feeds is available such

analysis could prove of value for complex problems. However, poorly chosen starting values can have a detrimental effect on the convergence of a process simulation.

More recently, K. Lee (7) formulates the selection of process equipment and the subsequent integration of the flowsheet into a linear programming problem. By use of the branch and bound method of solving integer programming problems, (a method of linear programming), Lee seeks to optimize a heat exchanger network based on equipment cost. Difficulties arise when uncalculable parameters such as fouling factors share control of the actual operation of all process equipment. Ultimately, if all design problems could be carefully formulated in terms of design variables and other factors such as improved correlations for true heat transfer coefficients, the solution of multiple nonlinear equations could replace some of the artistry of design. However, so many physical properties and mechanical problems are so poorly defined in the current state of the art that much of design must be based on previous success. As design engineers receive better prediction methods for physical properties and design variables, the optimization procedures may become of greater value.

CHAPTER III

PROCEDURE

One of the difficulties individuals such as Kliesch encounter in evaluating recycle acceleration techniques is the creation of a satisfactory simulation system to handle the recycle problem. At Oklahoma State University, Erbar (2) has developed a chemical process simulation system for hydrocarbons and related compounds. Contained in the system are the following modules: adder, divider, compressor, pump, flash, heat exchanger, distillation column, and absorber. The OSUPAS system, depending on the form of recycle acceleration, requires between 190K and 380K in the "link edit" step on the IBM 360/65 computer belonging to Oklahoma State University. To facilitate a complete analysis of results, both the processor time in the "go" step and the amount of storage required in the "go" step in each of the fourteen problems is reported.

Methods Tested

1. Successive substitutions is the standard solution technique used in the OSUPAS system. The technique involves the substitution of a calculated value for a recycle stream vector in place of the previously assumed (or calculated) value of the vector at each recycle entry point.

2. An exponential model is attempted in two versions. The basic
form of the model in either case is shown in Equation (35).

$$X_i = \alpha_i \ (1-e^{-An})$$ (35)

In the first case the values of α and A are determined by the method of
Isakson (3) on an independent componential basis. The other form
utilizes empirically fitted values of A on the total stream molar
flow rate.

3. The Bounded Wegstein method is tested to determine the useful-
ness of the approach over a broad range of applications. Because of
difficulties with oscillation, application of the method is initially
deferred for three iterations as suggested by Kliesch. The method is
then applied on alternate iterations to suppress oscillation. Subse-
quent tests, including the criterion developed at the end of this
section, reduce the degree of oscillation that is inherently present
in the convergence pattern of the algorithm by the introduction of an
application parameter.

4. The split fraction approach of Rosen (15), is implemented to
test the effect of a closed material balance on the rate of conver-
gence acceleration of the system. The procedure is developed for
Problem 7, Figure 16 and although other systems are examined with the
procedure, the internal function is only verified for the original
problem.

5. The split fraction approach is then coupled with the Bounded
Wegstein algorithm to accelerate the final value determination of the
split fractions.

Problems

The problems are examined insofar as possible by the methods mentioned to compare convergence patterns. Figures 10 to 22 contain the flowsheets and design variable specifications. Some of the problems are of no industrial importance. These are used either to illustrate an extreme (no variable interaction) case as in Problem 11, or to serve as a basis of comparison with previous work as in Problem 7. Each problem assumes a zero starting value for all elements in the recycle stream vector, except for Problems 5 and 6. Additional design variable specifications are shown in Tables I through XIII.
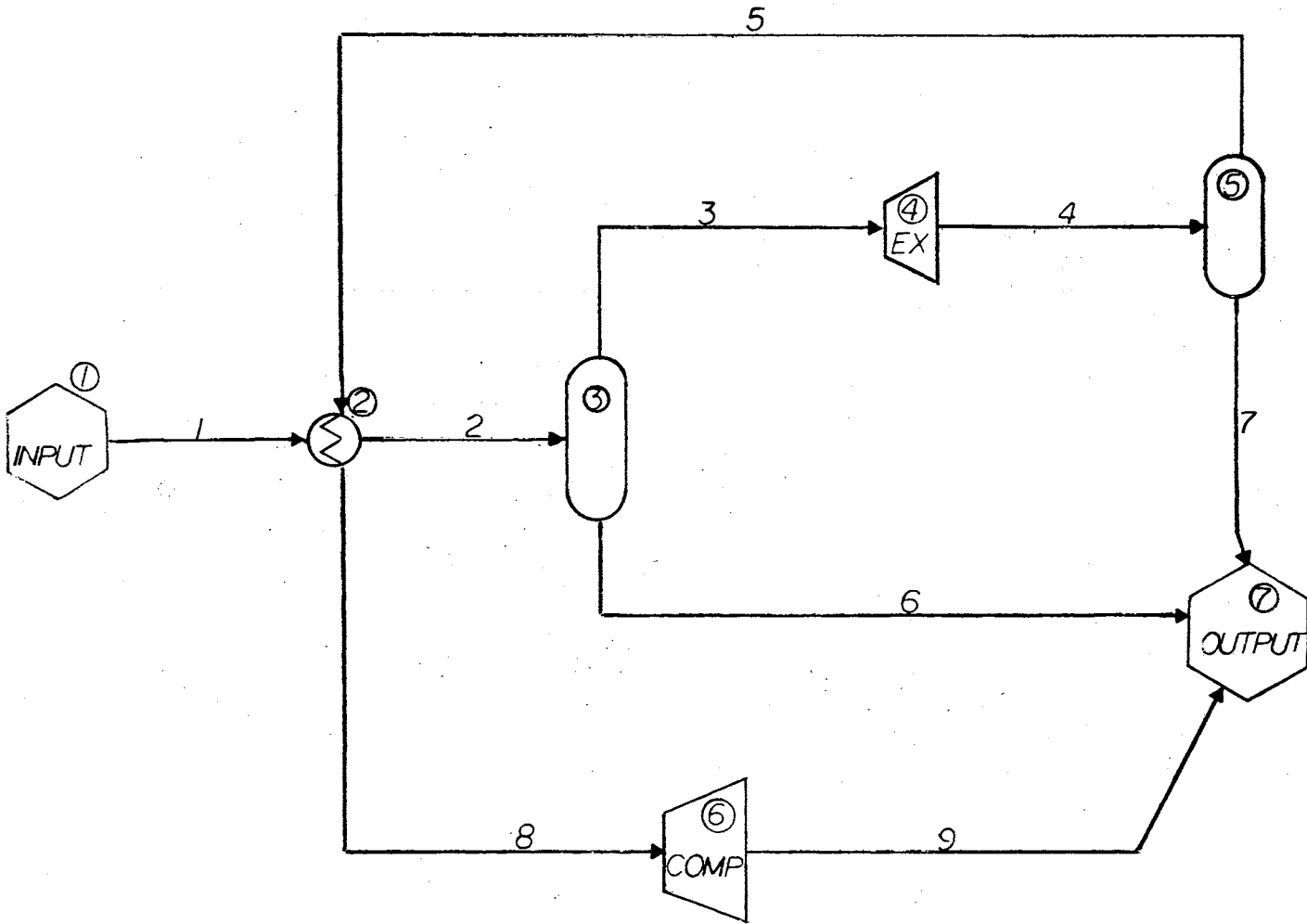
Figure 10. Schematic Flow Design of Compressor-Expander (Problem No. 1)

TABLE I

PROCESS SPECIFICATIONS FOR THE
COMPRESSOR-EXPANDER PROBLEM

Process Description

2 - Heat Exchanger	3 - Flash	4 - Expander	5 - Flash	6 - Compressor
Approach = 10°F Pressure drop on either side = 5 psia	Pressure = 245 psia	Discharge pressure = 80 psia Efficiency = 60%	Pressure = 80 psia	Discharge pressure = 98 psia Efficiency = 55%

Feed Stream 1

Temperature = 95°F   Pressure = 250 psia

Component	Moles/hr
Methane	5900.0
Ethane	410.0
Propane	160.0
i-Butane	30.0
n-Butane	45.0
i-Pentane	9.0
n-Pentane	15.0
n-Heptane	5.0
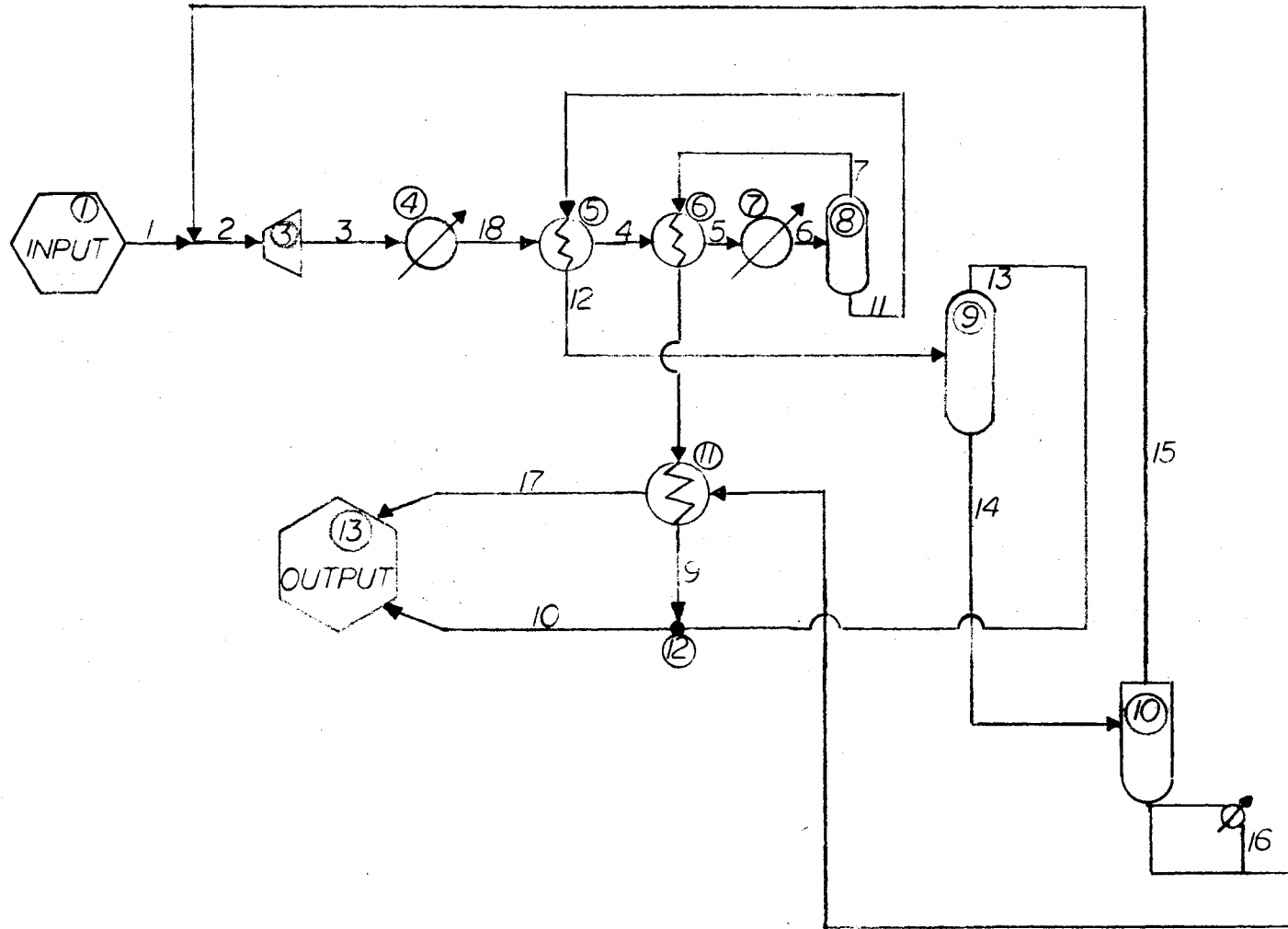
Figure 11. Schematic Flow Design of Cavett's Second Problem (Problem No. 2)

TABLE II

PROCESS SPECIFICATIONS FOR CAVETT'S SECOND PROBLEM

Process Description

3 - Compressor	4 - Heat Exchanger	5 - Heat Exchanger	6 - Heat Exchanger	7 - Heat Exchanger	8 - Flash	9 - Flash	10 - Stabilizer	Exchanger
Discharge pressure = 400 psia Efficiency = 60%	Outlet temperature = 70°F Pressure drop = 2 psi	Approach = 10°F Pressure drop = 30 psi	Approach = 10°F Pressure drop = 30 psi	Outlet temperature = 0°F Pressure drop = 2.0 psi	Tempera-ture = 0°F Pressure = 390 psia	Pressure = 300 psia	Pressure = 150 psia D/F = .82 Stage = 8 Tray Spacing = 24"	Approach = 1°F

TABLE II (Continued)

Feed Stream 1	
Temperature = 70°F	Pressure = 150 psia

Component	Moles/hr
Methane	8276.0
Ethane	871.0
Propane	411.0
i-Butane	28.0
n-Butane	113.0
i-Pentane	25.0
n-Pentane	32.0
n-Hexane	21.0
n-Heptane	12.0
Carbon Dioxide	20.0
Nitrogen	191.0
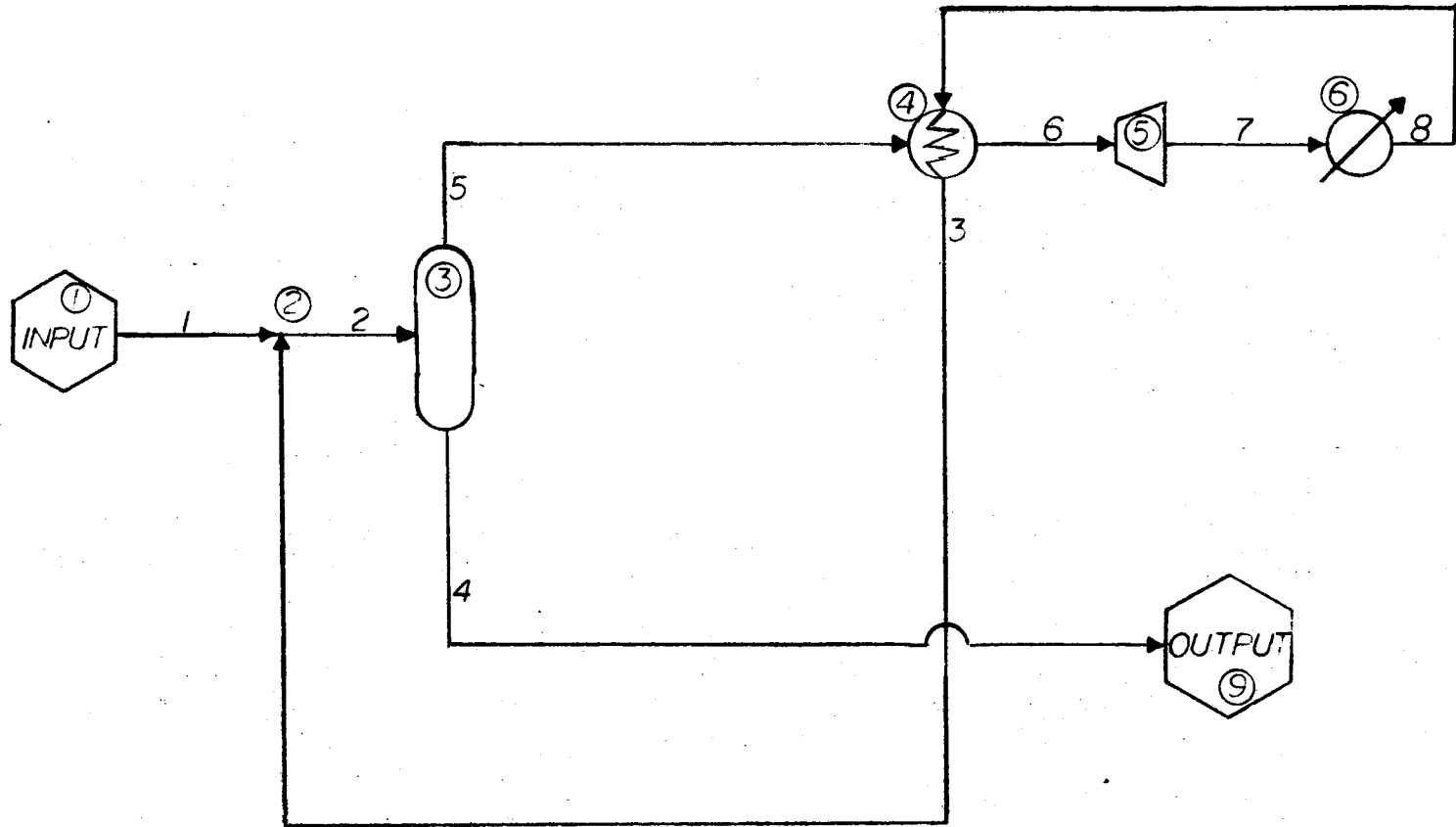
Figure 12. Schematic Flow Design of Olefin Tank Refrigeration (Problem No. 3)

TABLE III

PROCESS SPECIFICATIONS FOR
OLEFIN TANK REFRIGERATION

Process Description

3 - Flash	4 - Heat Exchanger	5 - Compressor	6 - Heat Exchanger
Pressure = 75 psia	Approach = 10°F Pressure drop = 2 psi	Discharge pressure = 260 psia Efficiency = 85%	Outlet temperature = 130°F

Feed Stream 1

Temperature = 105°F   Pressure = 200 psia

Component	Moles/hr
Propane	192.5
i-Butane	452.5
n-Butane	515.0
i-Pentane	505.0
Propylene	400.0
1 Butene	532.5
1 Pentene	267.5
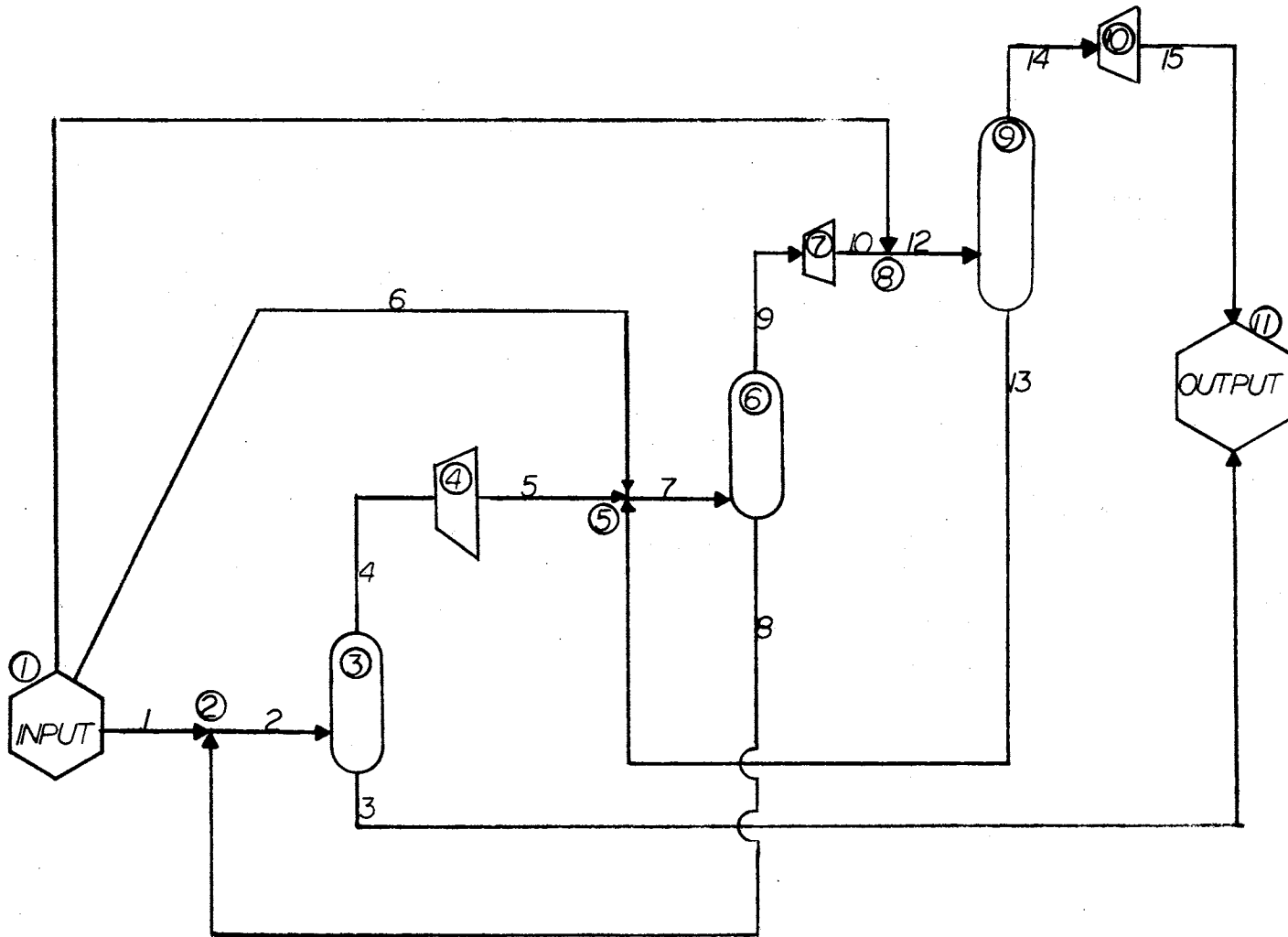
Figure 13.   Schematic Flow Design of a Recompression Plant (Problem No. 4)

TABLE IV

PROCESS SPECIFICATIONS FOR
A RECOMPRESSION PLANT

Process Description

3-Flash	4-Compressor	6-Flash	7-Compressor	9-Flash	10-Compressor
Temperature = 110°F Pressure = 30 psia	Discharge pressure = 90 psia Efficiency = 82%	Temperature = 110°F Pressure = 90 psia	Discharge pressure = 280 psia Efficiency = 82%	Temperature = 55°F Pressure = 280 psia	Discharge pressure = 1025 psia Efficiency = 82%

Feed Stream 1

Temperature = 110°F
Pressure = 30 psia

Feed Stream 6

Temperature = 100°F
Pressure = 90 psia

Feed Stream 11

Temperature = 55°F
Pressure = 280 psia

Component	Moles/hr	Component	Moles/hr	Component	Moles/hr
Nitrogen	0.0	Nitrogen	0.1	Nitrogen	0.33
Carbon Dioxide	0.1	Carbon Dioxide	0.9	Carbon Dioxide	2.93
Methane	5.1	Methane	73.4	Methane	185.33
Ethane	5.8	Ethane	20.1	Ethane	67.28
Propane	10.4	Propane	14.7	Propane	6.33
i-Butane	4.6	i-Butane	4.7	i-Butane	0.75
n-Butane	4.4	n-Butane	3.4	n-Butane	0.38
i-Pentane	1.8	i-Pentane	1.1	i-Pentane	0.04
n-Pentane	1.2	n-Pentane	0.6	n-Pentane	0.02
n-Heptane	1.8	n-Heptane	0.8	n-Heptane	0.00
n-Nonane	0.0	n-Nonane	0.0	n-Nonane	0.16
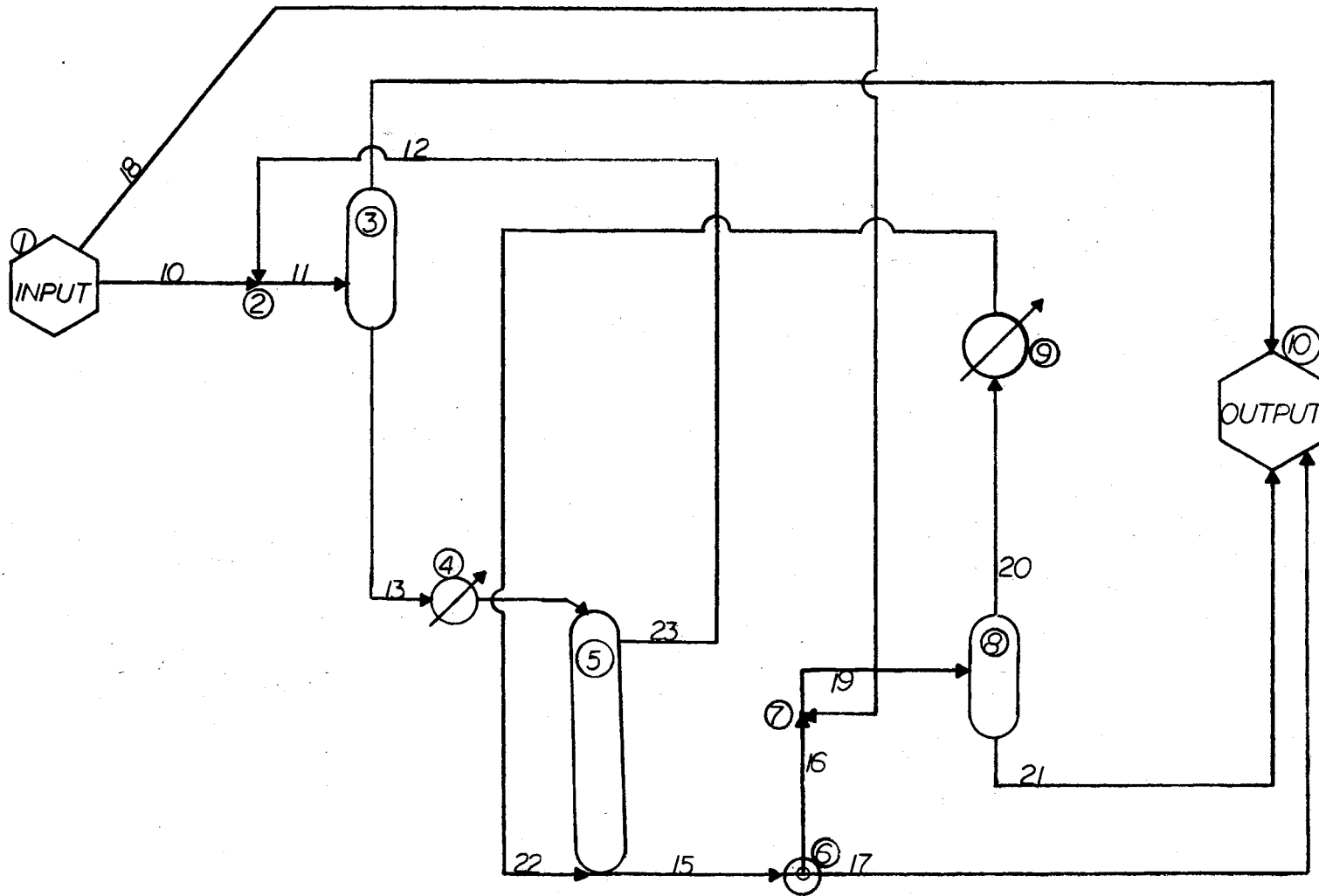
Figure 14. Schematic Flow Design of Absorber Network (Problem No. 5)

TABLE V

PROCESS SPECIFICATIONS FOR THE ABSORBER
NETWORK PROBLEM

Process Description

3-Flash	4-Heat Exchanger	5-Absorber	6-Splitter	8-Flash	9-Heat Exchanger
Temperature = $110°F$ Pressure = 544 psia	Outlet temperature = $233°F$	Stages = 4 Lean gas pressure = 620 psia Rich oil pressure = 624 psia Tray spacing = 24"	100% of heavy oil is sent to stream 17, the remainder of stream 15 is sent to stream 16	Temperature = $110°F$ Pressure = 324 psia	Outlet temperature = $231°F$

TABLE V (Continued)

Feed Stream 10		Feed Stream 18	
Temperature = $110^{\circ}F$		Temperature = $110^{\circ}F$	
Pressure = 544 psia		Pressure = 324 psia	

Component	Moles/hr	Component	Moles/hr
Hydrogen	0.0	Hydrogen	1994.5
Hydrogen Sulfide	22.0	Hydrogen Sulfide	0.0
Methane	0.0	Methane	330.5
Ethane	0.0	Ethane	249.7
Propane	0.0	Propane	248.7
i-Butane	0.0	i-Butane	78.6
n-Butane	2.2	n-Butane	129.1
Hypothetical Component *	1629.4	Hypothetical Component *	412.5

* Physical properties of hypothetical component -- NBPT = $240^{\circ}F$
  $^{\circ}API = 56.8$ Molecular Weight - 112.1
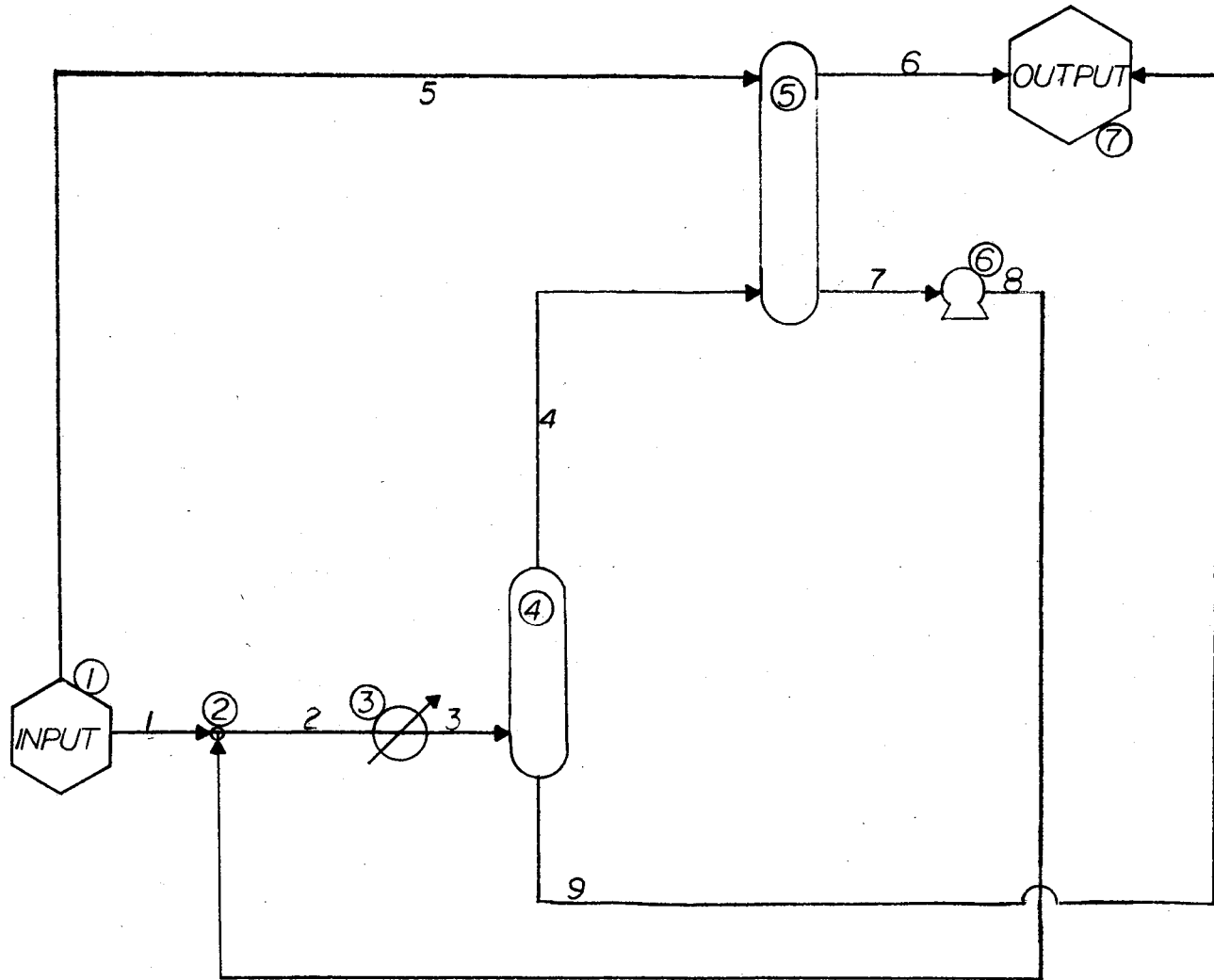
Figure 15. Schematic Flow Design of Gas Cleanup Before
Depropanization (Problem No. 6)

TABLE VI

PROCESS SPECIFICATIONS FOR GAS CLEANUP
BEFORE DEPROPANIZATION

Process Description

3-Heat Exchanger	4-Flash	5-Absorber	6-Pump
Outlet temperature = 100°F Pressure drop = 5 psi	Temperature = 100°F Pressure = 90 psia	Stages = 4 Lean gas pressure = 90 psia Rich oil pressure = 80 psia Tray spacing = 24"	Discharge pressure = 95 psia Efficiency = 60%

Feed Stream 1

Temperature = 120°F
Pressure = 111 psia

Feed Stream 5

Temperature = 100°F
Pressure = 80 psia

Component	Moles/hr	Component	Moles/hr
Methane	50.3	Methane	0.0
Ethane	78.4	Ethane	0.0
Propane	120.6	Propane	0.0
i-Butane	172.6	i-Butane	0.0
n-Butane	243.7	n-Butane	0.0
i-Pentane	5.1	i-Pentane	0.0
Hypothetical Component *	0.0	Hypothetical Component *	600.0

* Physical properties of hypothetical component -- NBPT = 270°F
   °API = 70.0   Molecular Weight = 130
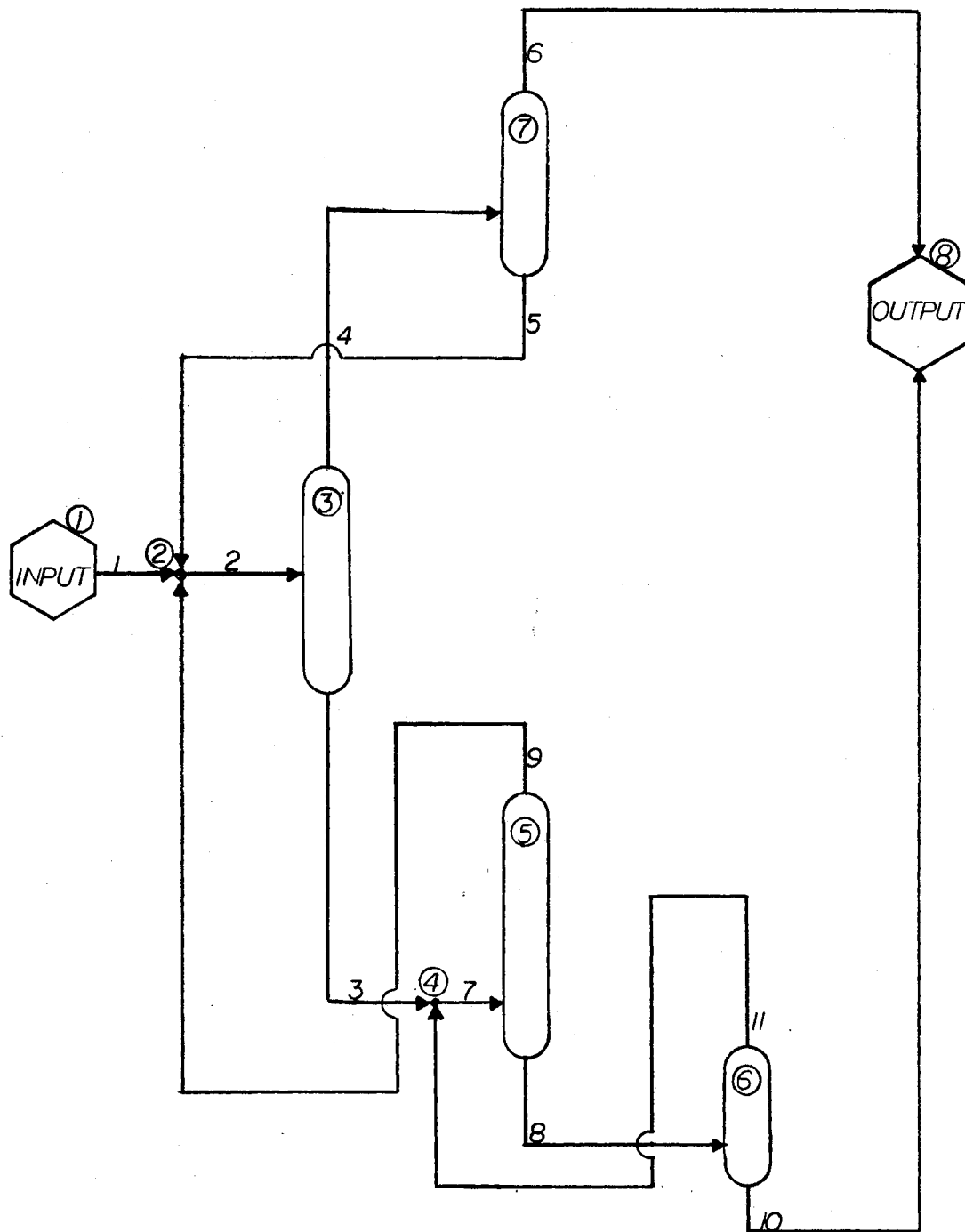
Figure 16. Schematic Flow Design of Cavett's First
Problem (Problem No. 7)

TABLE VII

PROCESS SPECIFICATIONS FOR
CAVETT'S FIRST PROBLEM

Process Description

3-Flash	5-Flash	6-Flash	7-Flash
Temperature $= 120^{\circ}F$ Pressure = 270 psia	Temperature $= 96^{\circ}F$ Pressure = 49 psia	Temperature $= 85^{\circ}F$ Pressure = 13 psia	Temperature $= 100^{\circ}F$ Pressure = 800 psia

Feed Stream 1

Temperature = $120^{\circ}F$ Pressure = 270 psia

| Component	Moles/hr
Nitrogen	358.2
Carbon Dioxide	4965.6
Hydrogen Sulfide	339.4
Methane	2995.5
Ethane	2395.5
Propane	2291.0
i-Butane	604.1
n-Butane	1539.9
i-Pentane	790.4
n-Pentane	1129.9
n-Hexane	1754.7
n-Heptane	2606.7
n-Octane	1844.5
n-Nonane	1669.0
n-Decane	831.7
n-Undecane	1214.5
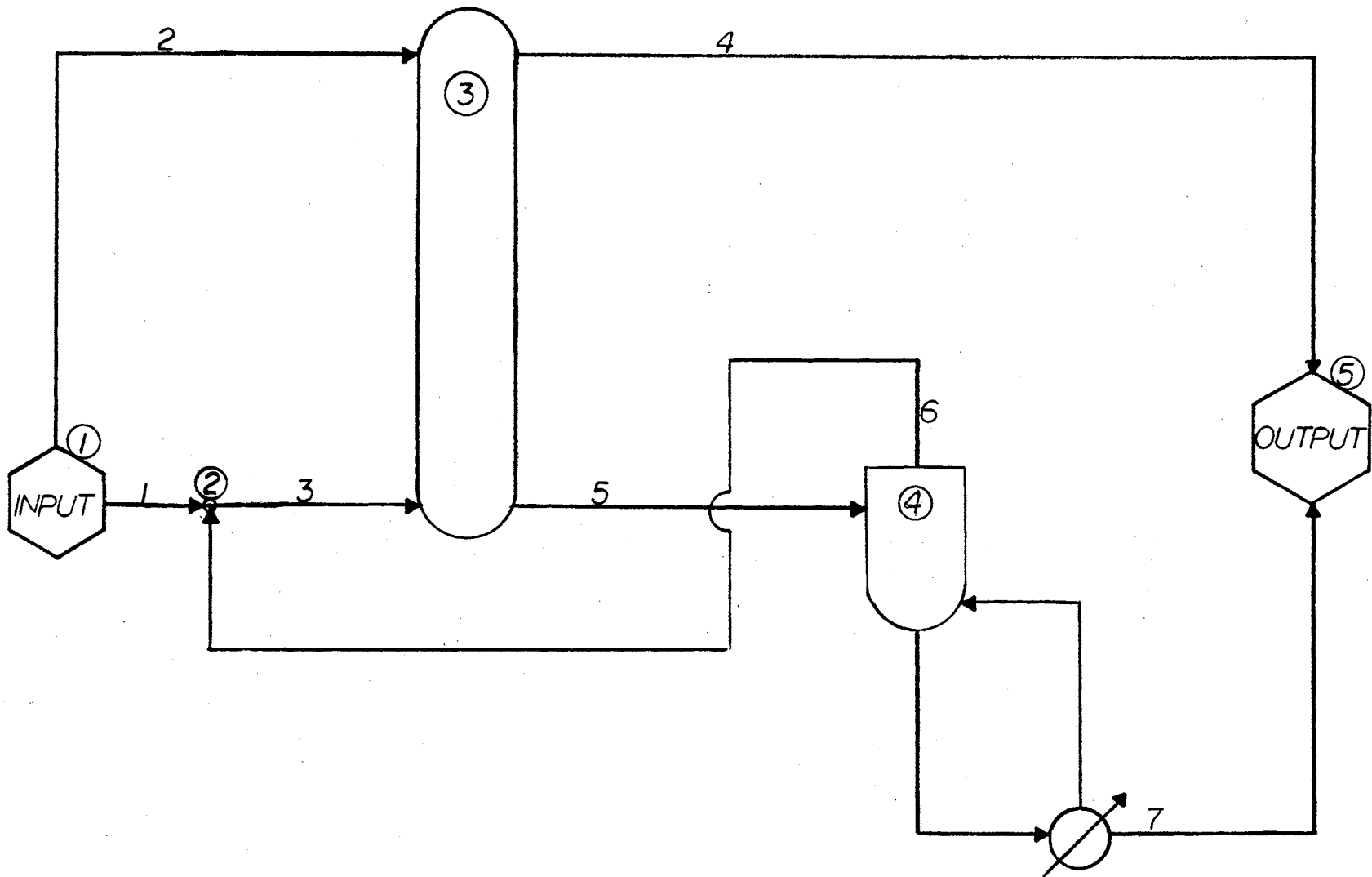
Figure 17. Schematic Flow Design of Absorber Problem (Problem Nos. 8 and 9)

TABLE VIII

PROCESS SPECIFICATIONS FOR
THE ABSORBER PROBLEM

Process Description
Problem No. 8
Lean Oil Rate Fixed

3-Absorber	4-Stabilizer
Stages = 7	Column pressure = 100 psia
Lean gas pressure = 96 psia	D/F = .15
Rich oil pressure = 98 psia	Stages = 6
$T_{LG}-T_{LO} = 15^{O}F$	Tray spacing = 24"

Process Description
Problem No. 9
Lean Oil Rate Calculated

3-Absorber	4-Stabilizer
Key component C_3	Column pressure = 100 psia
E_A = .90	D/F = .15
Stages = 7	Stages = 6
Lean gas pressure - 96 psia	Tray spacing = 24"
Rich oil pressure = 98 psia	
$T_{LG}-T_{LO} = 15^{O}F$	

TABLE VIII (Continued)

Feed Stream 1 Temperature = 100°F Pressure = 100 psia		Feed Stream 2 Temperature = 100°F Pressure = 100 psia	
Component	Moles/hr	Component	Moles/hr
Hydrogen	63.40	Hydrogen	0.00
Methane	119.60	Methane	0.00
Ethane	134.80	Ethane	0.00
Propane	90.56	Propane	0.00
i-Butane	11.30	i-Butane	0.00
n-Butane	29.30	n-Butane	0.00
i-Pentane	3.70	i-Pentane	0.00
n-Pentane	4.70	n-Pentane	0.00
Hydrogen sulfide	2.20	Hydrogen Sulfide	0.00
Hexane +*	9.30	Hexane	0.00
Hypothetical Component 1 *	0.00	Hypothetical Component 1 *	25.76
Hypothetical Component 2 *	0.00	Hypothetical Component 2 *	51.44
Hypothetical Component 3 *	0.00	Hypothetical Component 3 *	77.10
Hypothetical Component 4 *	0.00	Hypothetical Component 4 *	102.81
Hypothetical Component 5*	0.00	Hypothetical Component 5*	257.02
Hypothetical Component 6 *	0.00	Hypothetical Component 6 *	154.24
Hypothetical Component 7 *	0.00	Hypothetical Component 7 *	102.87

* Physical properties of the hypothetical components --

Component	NBPT	°API	Mol. Wt.
Hexane +	136°F	89.8	80.0
Hypotehtical Component 1	162°F	80.2	93.0
Hypothetical Component 2	197°F	71.9	98.0
Hypothetical Component 3	213°F	66.5	104.0
Hypothetical Component 4	234°F	62.1	110.0
Hypothetical Component 5	259°F	57.9	116.0
Hypothetical Component 6	291°F	52.4	124.0
Hypothetical Component 7	338°F	45.4	137.0
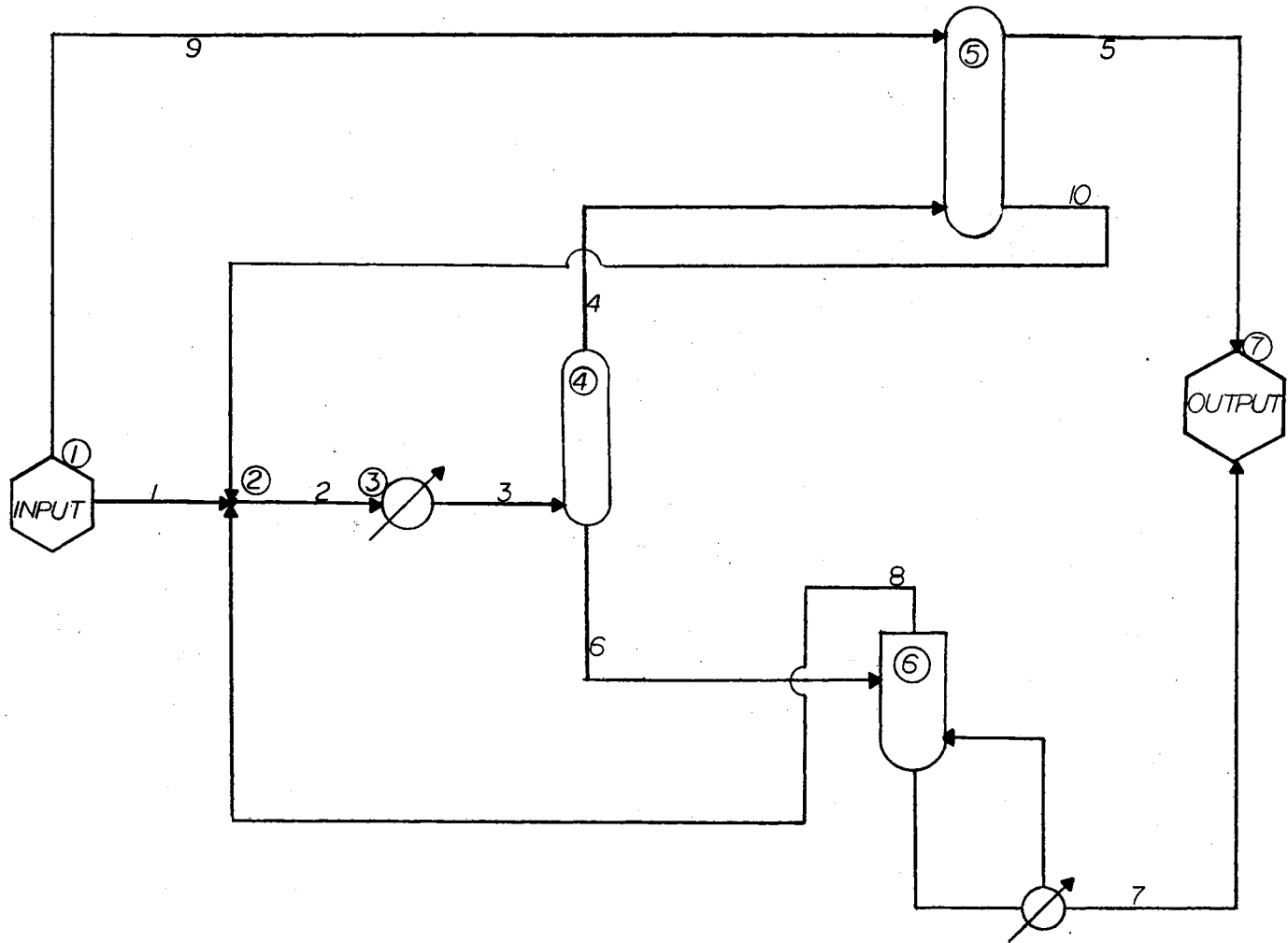
Figure 18.   Schematic Flow Design of Complete Stripper Absorber
System (Problem No. 10)

TABLE IX

PROCESS SPECIFICATIONS FOR THE COMPLETE
STRIPPER ABSORBER SYSTEM

Process Description

3-Heat Exchanger	4-Flash	5-Absorber	6-Stabilizer
Outlet temperature = 100°F Pressure drop - 5 psi	Temperature = 100°F Pressure = 90 psia	Stages = 4 Lean gas pressure = 90 psia Rich oil pressure = 80 psia Tray spacing = 24"	Column pressure = 95 psia D/F = .20 Stages = 6 Tray spacing = 24"

Feed Stream 1

Temperature = 120°F
Pressure = 11 psia

Feed Stream 9

Temperature = 100°F
Pressure = 80 psia

Component	Moles/hr	Component	Moles/hr
Methane	50.3	Methane	0.0
Ethane	78.4	Ethane	0.0
Propane	120.6	Propane	0.0
i-Butane	172.6	i-Butane	0.0
n-Butane	243.7	n-Butane	0.0
i-Pentane	5.1	i-Pentane	0.0
Hypothetical Component 1 *	0.0	Hypothetical Component 1 *	600.0

* Physical properties of hypothetical component -- NBPT = 270°F
$^\circ$API = 70   Molecular Weight = 130
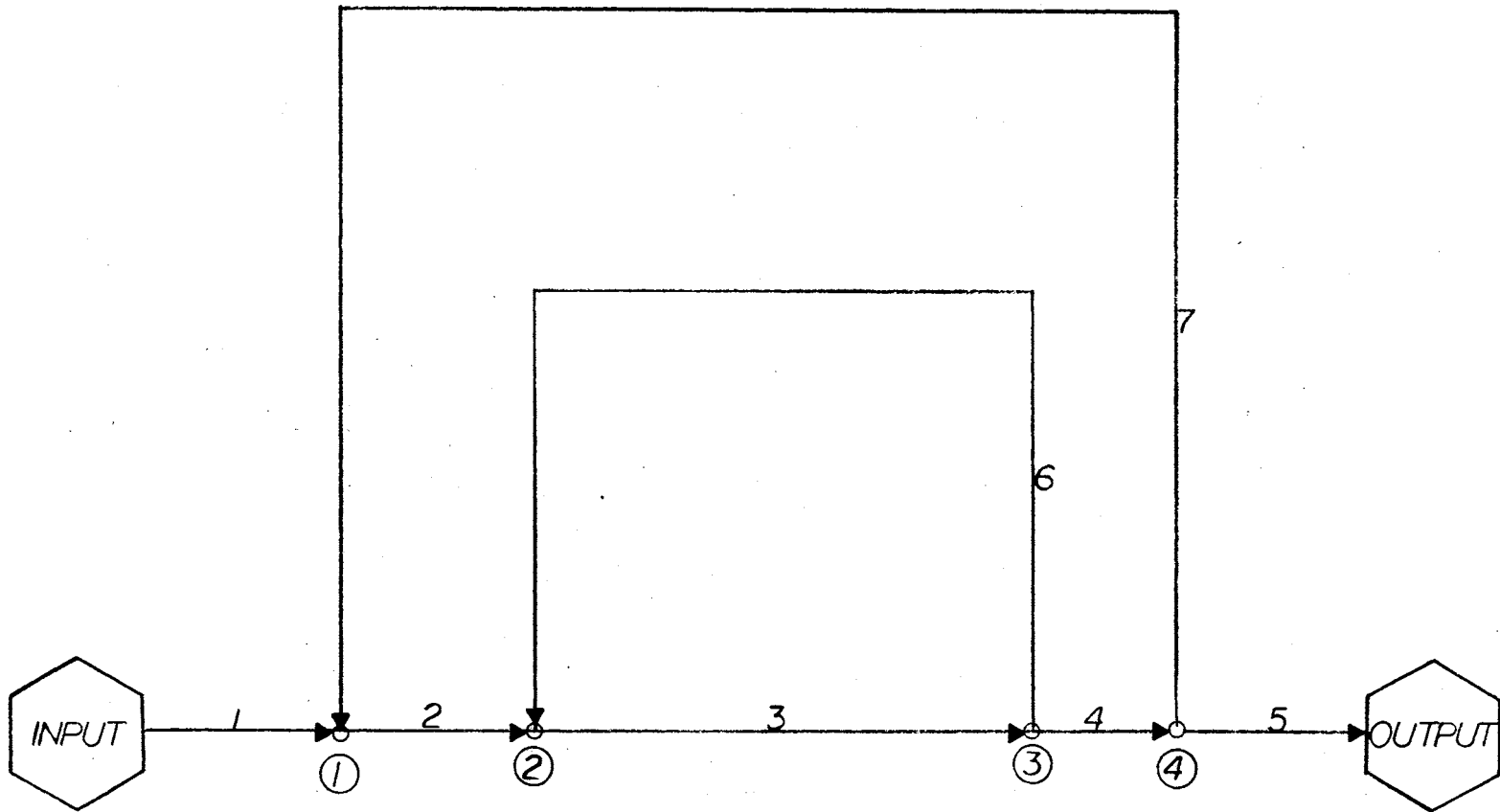
Figure 19.   Schematic Flow Design of Adder-Divider Problem (Problem No. 11)

TABLE X

PROCESS SPECIFICATIONS FOR THE
ADDER-DIVIDER PROBLEM

Process Description

3-Divider	4-Divider
50% to stream 6	10% to stream 5
50% to stream 4	90% to stream 7

Feed Stream 1

Temperature = $120^{\circ}F$ Pressure = 270 psia

Component	Moles/hr
Nitrogen	358.2
Carbon Dioxide	4965.6
Hydrogen Sulfide	339.4
Methane	2995.5
Ethane	2395.5
Propane	2291.0
i-Butane	604.1
n-Butane	1539.9
i-Pentane	790.4
n-Pentane	1129.9
n-Hexane	1764.7
n-Heptane	2606.7
n-Octane	1844.5
n-Nonane	1669.0
n-Decane	831.7
n-Undecane	1214.5

Figure 20. Schematic Flow Design of the Adder-Divider Form of Cavett's
First Problem (Problem No. 12)

TABLE XI

PROCESS SPECIFICATIONS FOR THE BENZENE
REACTOR WITH RECYCLE PROBLEM

Process Description

3-Reactor	4-Heat Exchanger	5-Flash	6-Splitter
Conversion - 50%	Outlet temperature = 70°F	Temperature - 70°F	10% to stream 7
Temperature = 1300°F		Pressure - 500 psia	90% to stream 9

Feed Stream 1

Temperature - 1500°F
Pressure - 500 psia

Feed Stream 8

Temperature - 1500°F
Pressure - 500 psia

Component	Moles/hr	Component	Moles/hr
Hydrogen	0.0	Hydrogen	25.0
Toluene	20.0	Toluene	0.0
Benzene	0.0	Benzene	0.0
Methane	0.0	Methane	0.0
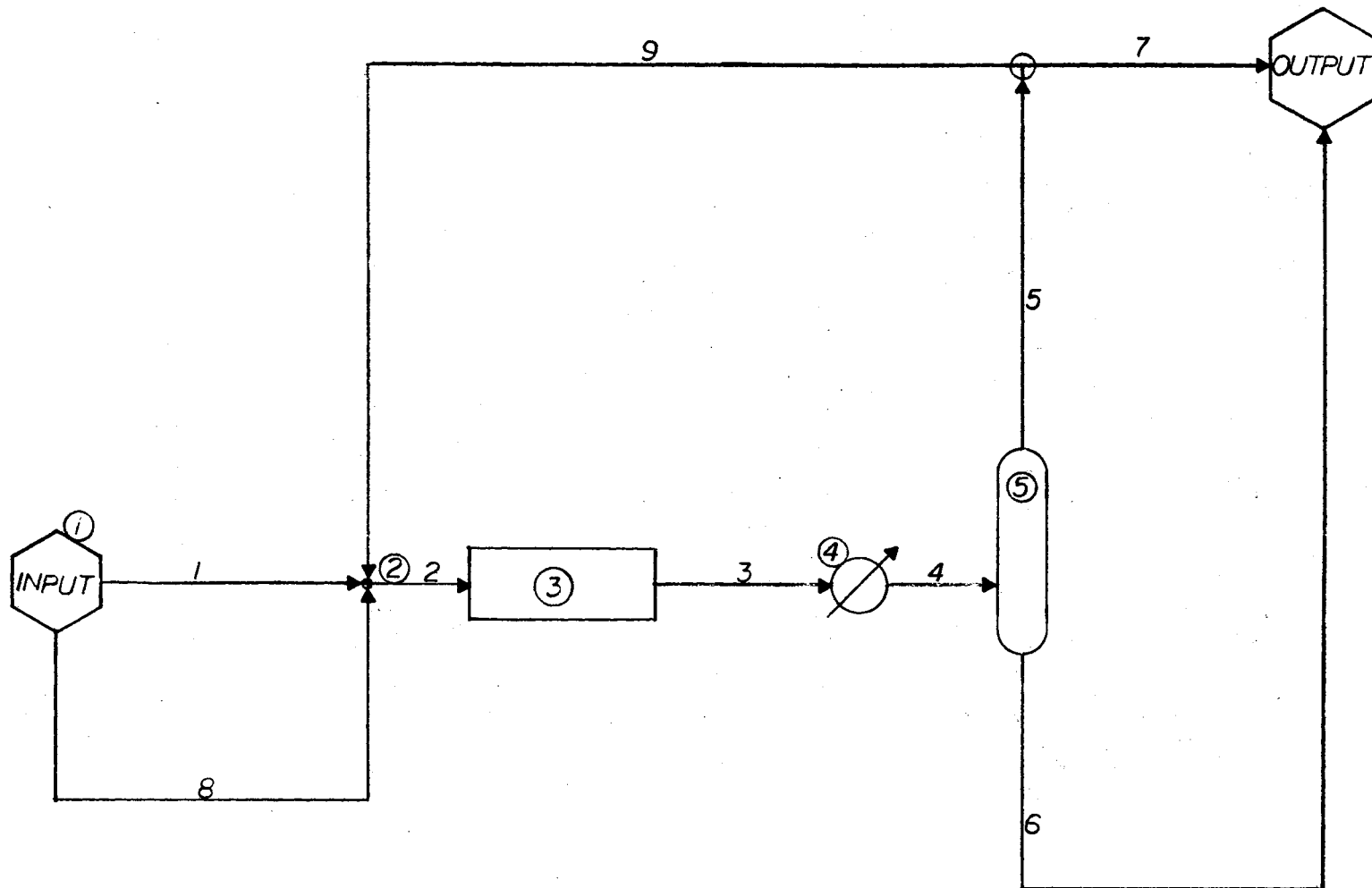
Figure 21. Schematic Flow Design of the Benzene Reactor with Recycle (Problem No. 13)

TABLE XII

PROCESS SPECIFICATIONS FOR THE ADDER-DIVIDER
FORM OF CAVETT'S FIRST PROBLEM

Process Description

3-Divider	5-Divider	6-Divider
59.2% to stream 3	39.3% to stream 10	27.8% to stream 11
40.8% to stream 7	60.7% to stream 5	72.2% to stream 6

Feed Stream 1

Temperature - 120°F   Pressure - 270 psia

Component	Moles/hr
Nitrogen	358.2
Carbon Dioxide	4965.6
Hydrogen Sulfide	339.4
Methane	2995.5
Ethane	2395.5
Propane	2291.0
i-Butane	604.1
n-Butane	1539.9
i-Pentane	790.4
n-Pentane	1129.9
n-Hexane	1764.7
n-Heptane	2606.7
n-Octane	1844.5
n-Nonane	1669.0
n-Decane	831.7
n-Undecane	1214.5
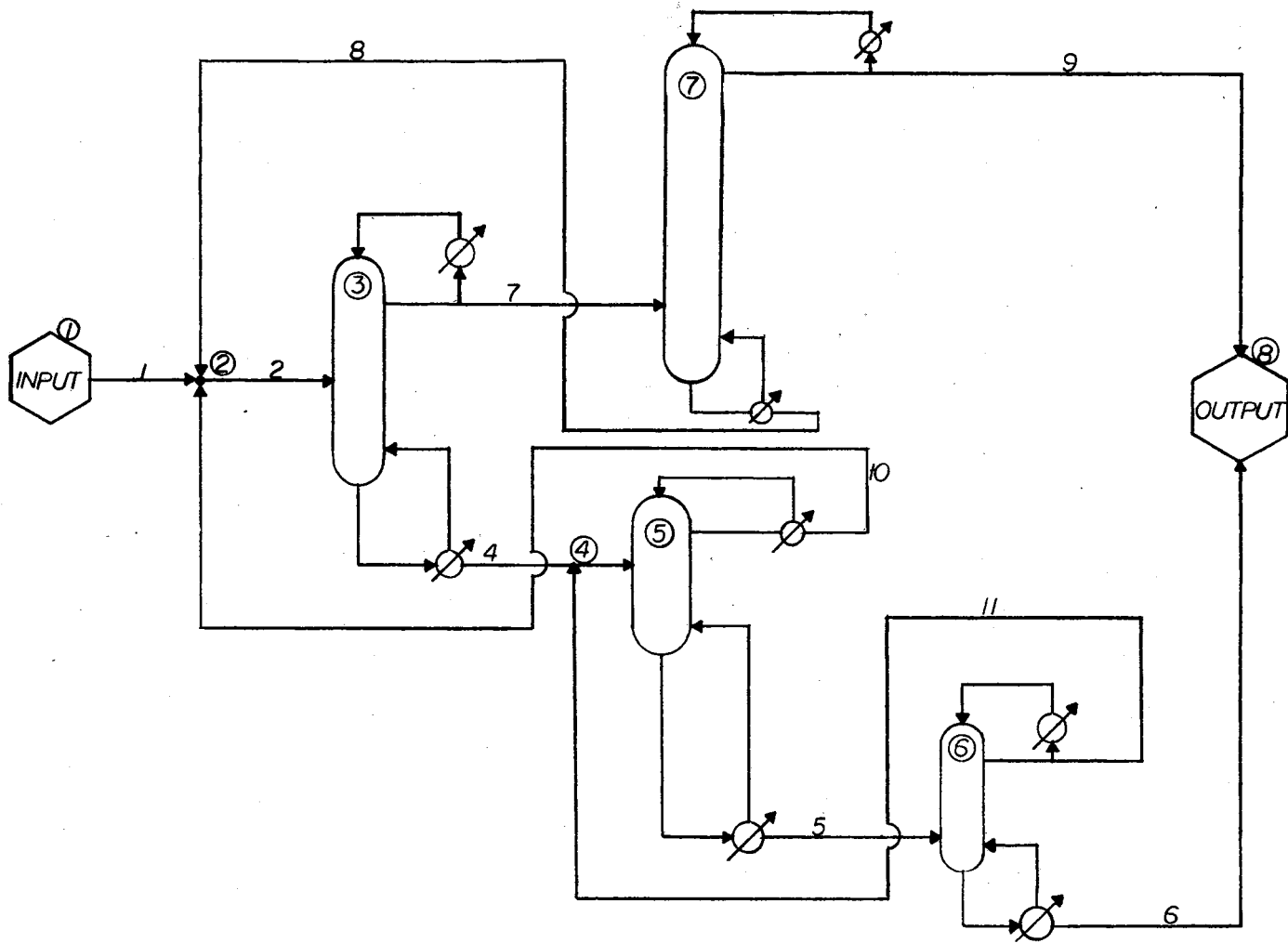
Figure 22.   Schematic Flow Design of the Distillation Form of Cavett's
First Problem (Problem No. 14)

TABLE XIII

PROCESS SPECIFICATIONS FOR THE DISTILLATION
FORM OF CAVETT'S FIRST PROBLEM

Process Description			
3-Distillation Unit	5-Distillation Unit	6-Distillation Unit	7-Distillation Unit
Pressure = 270 psia	Pressure = 49 psia	Pressure = 13 psia	Pressure = 800 psia
Light key C_2	Light key C_3	Light key iC_4	Light key C_3
Heavy key C_3	Heavy key iC_4	Heavy key – nC_4	Heavy key iC_4
$(d/b)_{LK} = 1.83$	$(d/b)_{LK} = 2.12$	$(d/b)_{LK} = 1.60$	$(d/b)_{LK} = 1.53$
$(b/d)_{HK} = 1.54$	$(b/d)_{HK} = 1.15$	$(b/d)_{HK} = .855$	$(b/d)_{HK} = 1.06$
Tray spacing = 24"	Tray spacing = 24"	Tray spacing = 24"	Tray spacing = 24"

TABLE XIII (Continued)

Feed Stream 1	
Component	Moles/hr
Nitrogen	358.2
Carbon Dioxide	4965.6
Hydrogen Sulfide	339.4
Methane	2995.5
Ethane	2291.0
Propane	604.1
i-Butane	1539.9
n-Butane	790.4
n-Pentane	1129.9
n-Hexane	1764.7
n-Heptane	2606.7
n-Octane	1844.5
n-Nonane	1669.0
n-Decane	831.7
n-Undecane	1214.5

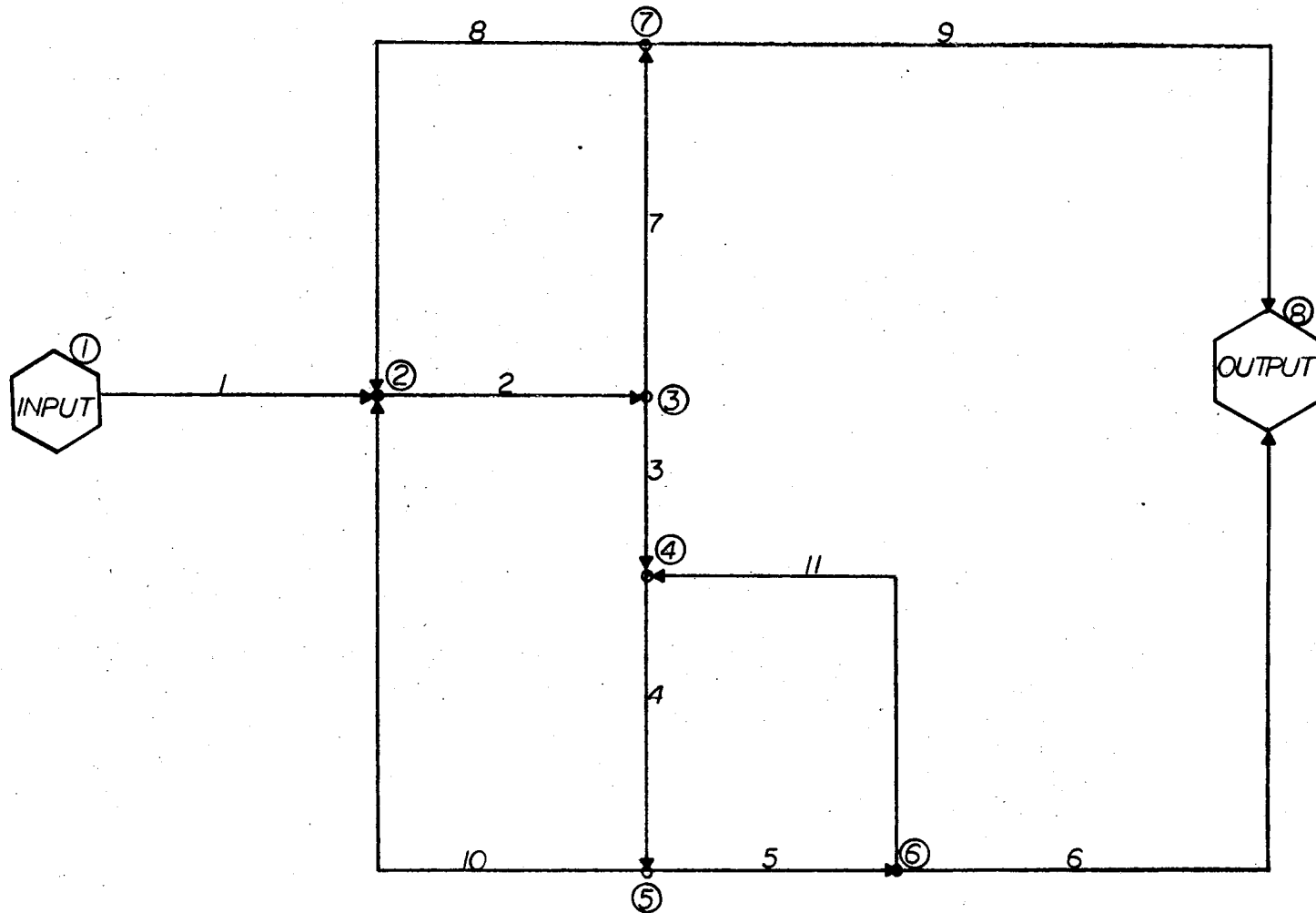## Criterion for Variable Interaction

Numerous authors (1, 4, 12, 17) have discussed variable interaction. Apparently, the only way to characterize this concept is by means of the flow rate interaction. If the flow rate of the major component is changed by an incremental amount, does a change in the flow rate for the other components occur? If no effect is noted on the other components, then the approximated derivative is the same as the total derivative of the function. Beginning with the successive substitution algorithm, an interaction criterion is developed in Equations (36) through (39).

$$\overline{X} = \overline{f}(\overline{X}) \tag{36}$$

$$X_{i+1,j} = f(X_{i1,i2, \ldots\ldots\ldots X_{ik}}) \tag{37}$$

$$df_j = \frac{\partial f_j}{\partial X_1} dX_1 + \frac{\partial f_j}{\partial X_2} dX_2 + \ldots \frac{\partial f_k}{\partial X_k} dX_k \tag{38}$$

$$\frac{df_j}{dX_j} = \frac{\partial f_j}{\partial X_1}\frac{dX_1}{dX_j} + \frac{\partial f_j}{\partial X_2}\frac{dX_2}{dX_j} + \cdots \frac{\partial f_k}{\partial X_k}\frac{dX_k}{dX_j} \tag{39}$$

$$C = \frac{\dfrac{df_j}{dX_j} - \dfrac{\partial f_j}{\partial X_j}}{\dfrac{df_j}{dX_j}} = 1 -$$

$$\tag{40}$$

$$\frac{\dfrac{\partial f_i}{\partial X_j}}{\dfrac{\partial f_j}{\partial X_1}\dfrac{dX_1}{dX_j} + \dfrac{\partial f_j}{\partial X_1}\dfrac{dX_2}{dX_j} + \cdots \dfrac{\partial X_i}{\partial X_j} \cdots + \dfrac{\partial f_j}{\partial X_k}\dfrac{dX_k}{dX_j}}$$

Obviously, $\dfrac{\partial f_k}{\partial X_j}$ for $k \neq j$ and $\dfrac{dX_i}{dX_k}$ again for $k \neq j$ will be zero if the variables are independent. Therefore, C is zero for the case of no interaction. As the interaction grows, the absolute value of C rises to a value that is some measure of the amount of interaction.

General

In summary, the objective of this work is to solve some trial recycle problems by various recycle convergence procedures and compare the effectiveness of the methods. From the comparison, a method is developed in the Results section which includes an application parameter or set of rules for the most effective means (in terms of time and storage commitments) to solve the recycle loop to a value of $\Delta_{imax} <$ 0.001. This comparison is in terms of the OSUPAS system. Other simulation systems may differ in internal tolerances (of heat balances and equilibrium convergence) and physical property evaluations, thereby altering the specific results. However, the same general characteristics are likely to be observed for any similar simulation system.

CHAPTER IV

RESULTS

The overall objective of this work is to provide an acceleration technique that will produce good acceleration when in the range of applicability and not damage convergence when out of this range. Factors such as the number of iterations for closure, size of the recycle stream, and variable interaction govern the range of applicability. The algorithms tested demonstrate a broad spectrum of reactions to various process applications. The results of all simulations are tabulated in Table XIV.

Successive Substitutions

In all cases tested, successive substitutions gives the same convergence pattern. An essentially monotonic sequence is generated that closed rapidly on the solution at first then gradually slows around the solution point until the step length (difference between vectors during successive iterations) becomes the same order of magnitude as the tolerance. Also the step lengths are seen to decay very slowly indicating that a large tolerance could yield an answer that differs from the true answer by more than the magnitude of the specified tolerance. No oscillatory behavior is observed and except for the number of iterations involved, the scheme is universally successful.

TABLE XIV

ITERATIONS, TIME, AND CORE COMPARISON

Problem Number	Bounded Wegstein with Application Parameter of 0.2 Core Storage Req. = 194k		Successive Substitutions Core Storage Req. = 190k		One Dimensional Bounded Wegstein Core Storage Req. = 192k		Bounded Wegstein Core Storage Req. = 192k		Split Fractions Core Storage Req. = 210k		Split Fraction with Bounded Wegstein Core Storage Req. = 336k	
	Iterations	Time (sec)	Iterations	Time (sec)	Iterations	Time (sec)	Iterations	Time (sec)	Iterations	Time (sec)	Iterations	Time (sec)
1	7	30.8	7	31.7			7	30.5	18	82.3		
2	24	209.6	24	152.6			27_+	237.7	26	246.8		
3	10	33.9	10	37.5			15^+(os)		10	40.0		
4	13	85.6	16	103.3			9	61.8	19	132.2		
5	11	39.2	14	43.0	15	43.5	9	32.4				
6	8	30.1	8	28.4			9_+	32.6				
7	27	111.6	44	129.6	35	110.7	50^+(os)		17	135.9	12	71.2
8	6	53.2	6	50.74			5	47.4				
9	4	147.0	6	157.0			5	161.3				
10	11	51.95	12	53.7			11	53.3				
11	4	12.3	77	73.9	3	10.1	3	10.3	3	20.2		
12	11	62.9	44	179.3			3	19.4				
13	6	21.92	8	20.5			9	23.5	3	15.6		
14	10	254.0	21	481.2	21	344.7	15	316.3				

Exponential Factor

When beginning the study two cursory observations are made about the behavior of recycle convergence. First, the convergence pattern for successive substitutions appears to have the form of an exponential decay function. Secondly, the vector might best be scaled by one factor for all components. Both of these statements are wrong.

The exponential decay function is not closely approximated by the convergence pattern due to the very slow approach to the asymptotic limit as compared to the initial portion of the function. In Problem 7 the last forty of fifty total iterations are required to travel a distance about ten percent of the converged solution. In this region the improvement for each iteration approaches a small constant value. Clearly, this behavior is not represented by the exponential decay function. The form of Isakson (3) is tested and found to oscillate when applied to Problem 7. Out of curiosity, arbitrary factors of A are tried for a constant scale factor for all variables. Strangely enough the constant scale factor does significantly improve convergence. This type of empiricism is constrained only to the tested Problem 7. Other attempts to use this form have been fruitless on other problems.

The concept of a constant acceleration factor for all variables is simply refuted by Figures 23 and 24 which show a monotonic increase for one variable and a general decrease for another variable in Problem 7. The most effective procedure is, therefore, a multicomponent adjustment on each step.
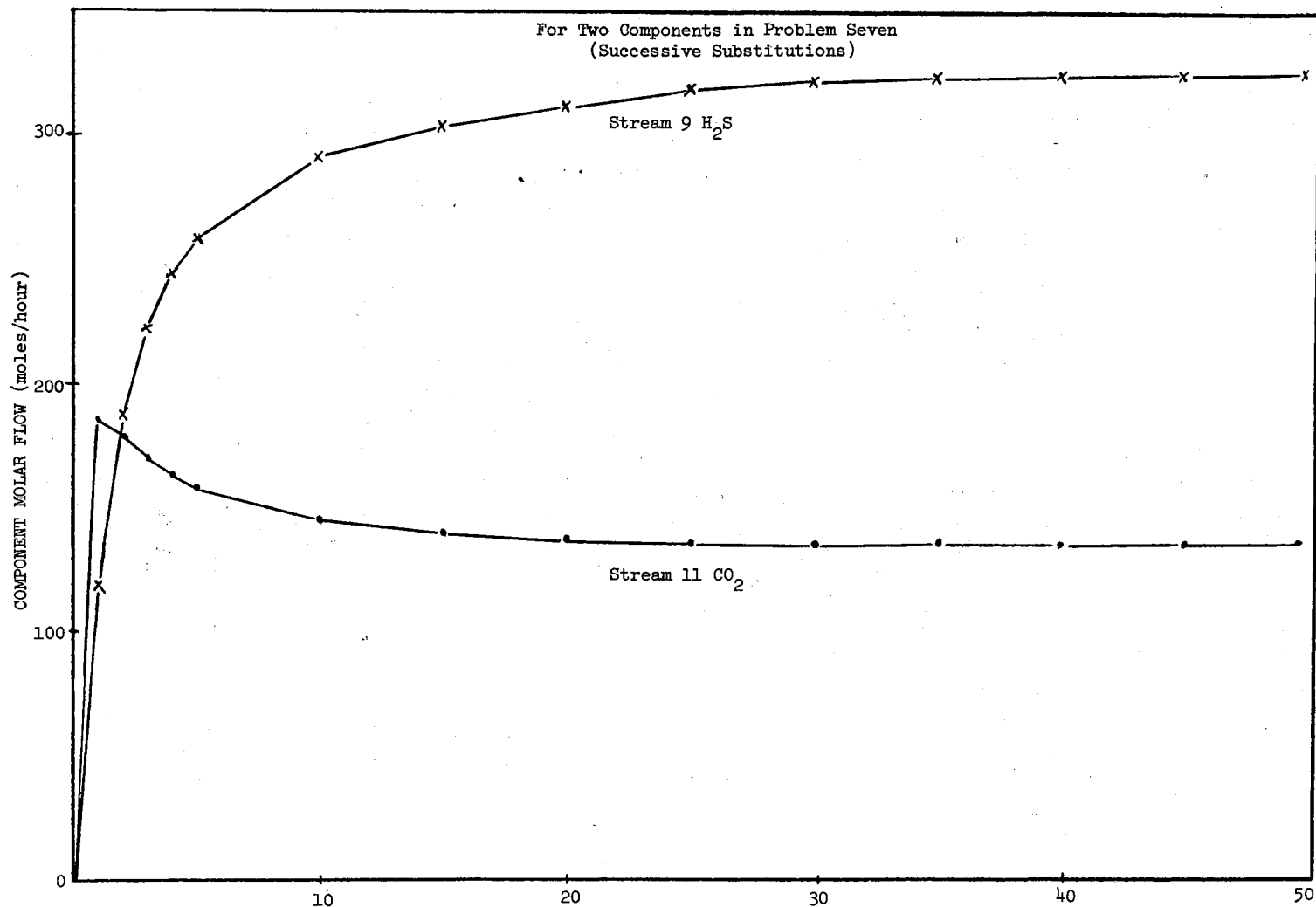
Figure 23. Comparison of Convergence Patterns
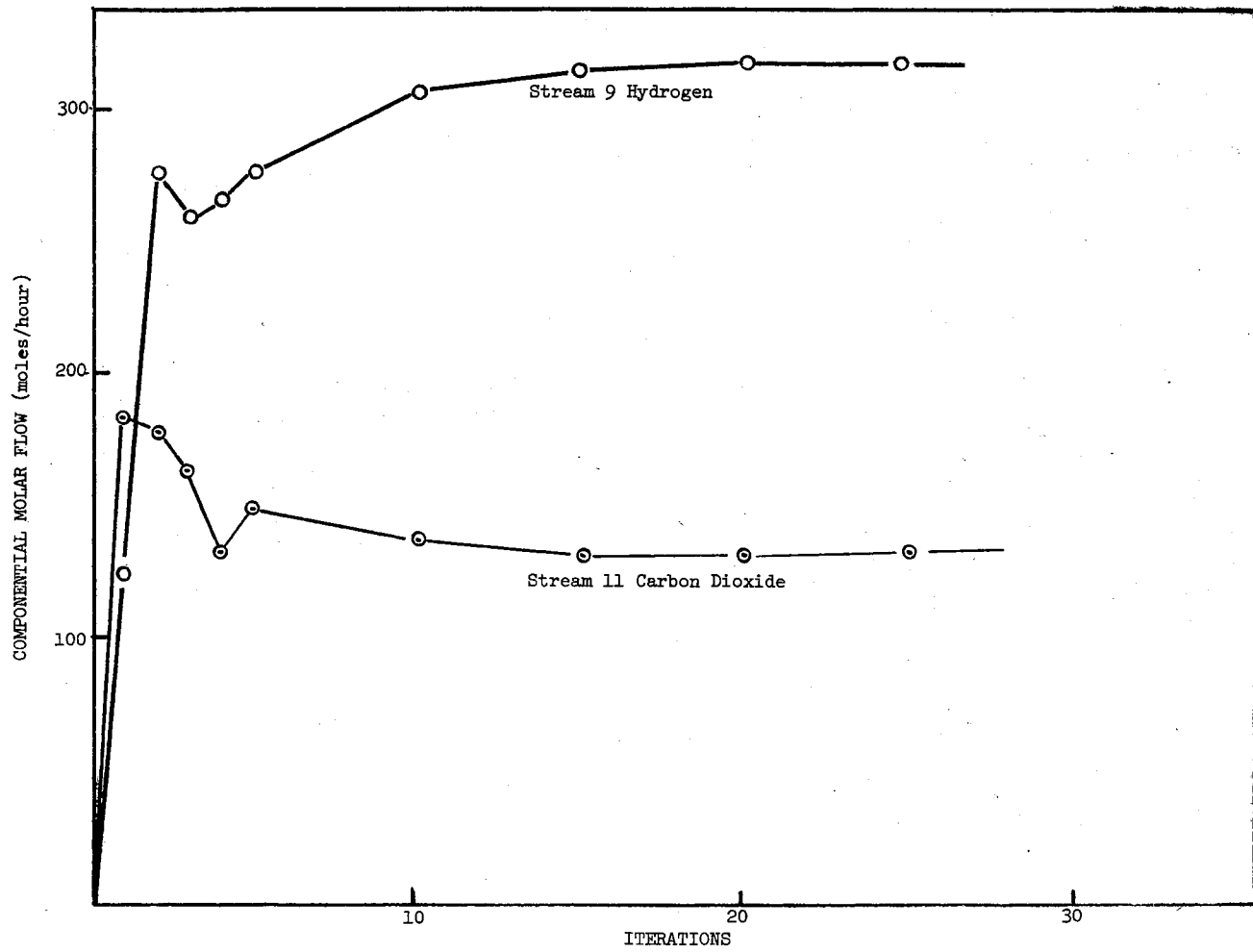
Figure 24. Comparison of Convergence Patterns for Two
Components in Problem Seven

Bounded Wegstein

The Bounded Wegstein procedure, is a multidimensional procedure which assumes the independence of variables. On cases like the synthetic adder-divider (Problem 11) where variable interaction does not exist, the Bounded Wegstein is rigorous within the computational accuracy of the computer. Additionally, a one dimensional Bounded Wegstein, based on total molar flow rate, is tested. The results, shown in Table XIV demonstrate the effectiveness of the Bounded Wegstein method as applied in this form. Difficulties arise in the applications of the multidimensional form to other cases. The solution pattern becomes more and more oscillatory as the variable interaction increases. Finally, the solution is hindered by the procedure (in some instances preventing solution). In order to suppress oscillation, many techniques have been attempted to determine when the acceleration step should be applied. Among the methods tested is the suppression of acceleration when the application parameter between iterations grows small as shown in Equation (41).

$$\text{application parameter} > \left\|\left\|\frac{X_{n+1}-X_n}{X_{n+1}}\right\|\right\| \quad \text{for each component of } \overline{X} \qquad (41)$$

This procedure has limited success but is difficult to generalize since a great number of iterations is required to close the last ten percent of the final solution of Problem 7. Many other techniques are attempted to bridge this problem without consistent success.

Orbach and Crowe (12) propose a reasonable application parameter in their paper. When successive values of the acceleration factor, λ,

are within 0.5% of one another, the acceleration procedure is repeated.
The factor λ is related (see page 21) to the componential derivative
of the stream vector. However, since the range of application of the
Bounded Wegstein techniques is governed by the amount of interaction,
the value of the bound on the Wegstein acceleration factor q should
be some function of the interaction criterion. Applying the inter-
action criterion (reference page 62) to several cases while determining
the optimal value of the bound, the criterion as presented is found
not to correlate with determined bound as shown in Figure 25. Logi-
cally the greater the interaction in each case the more tightly con-
strained the value of the bound must be. No generalizations to this
effect could be made from the available case information. Fortunately,
the well around the optimal value of the bound as shown by Figure 26
is relatively flat. This permits use of a bound that is not optimal
without having a significantly detrimental effect on the number of
iterations. By inspection of the results of several problems, a mean
value of 0.2 is chosen for the bound on the application of q shown in
Equation (42).

$$0.2 > \frac{q_{n+1} - q_n}{q_{n+1}} \quad \text{for each component of } \overline{X}_n \quad (42)$$

The constrained version of the Bounded Wegstein has the most general
range of application to all the test cases and also the best overall
time ratios of the general methods. A programming flow diagram is
presented on page 78 for the Bounded Wegstein with the application
parameter.
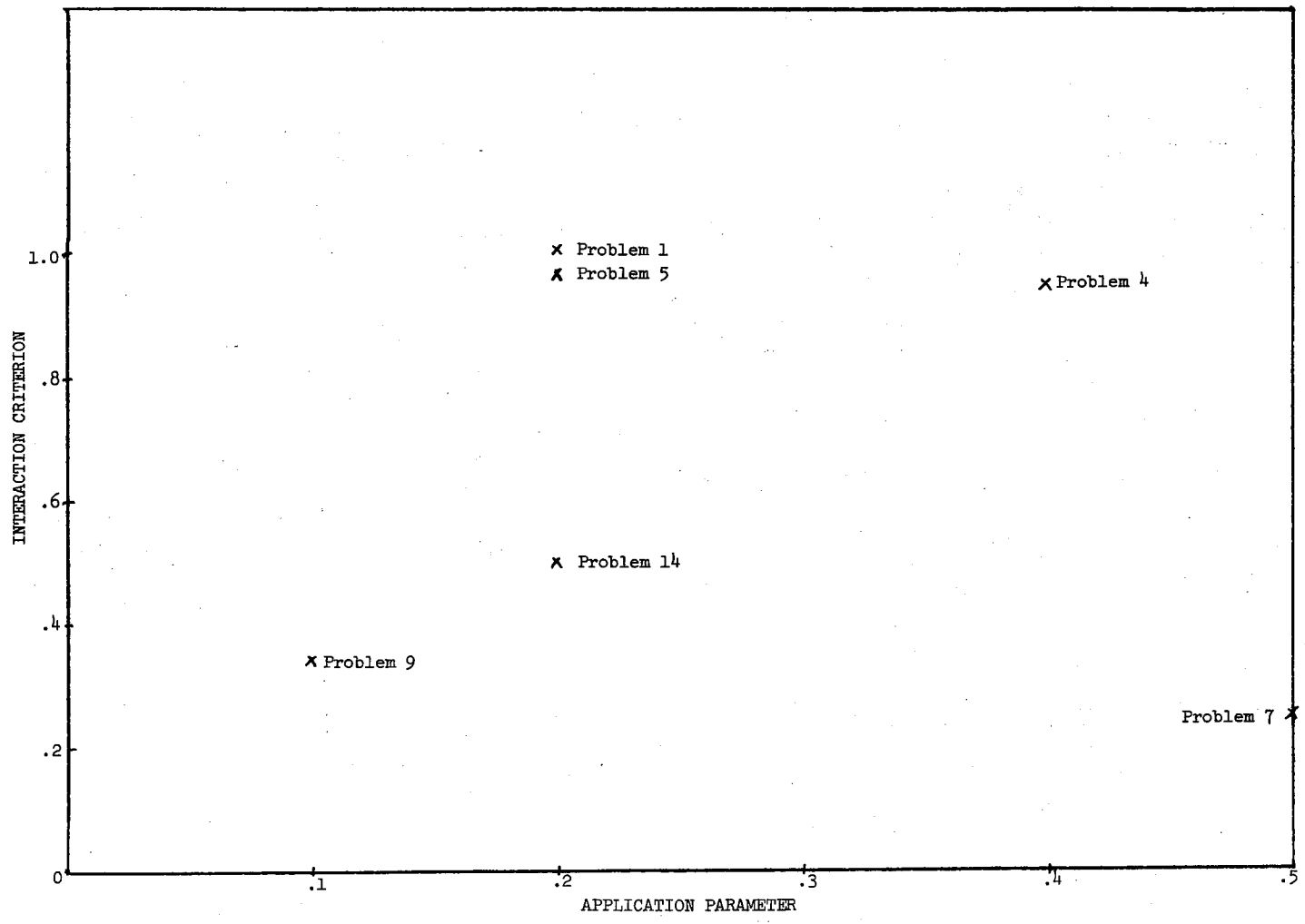
Figure 25. Optimal Application Parameters
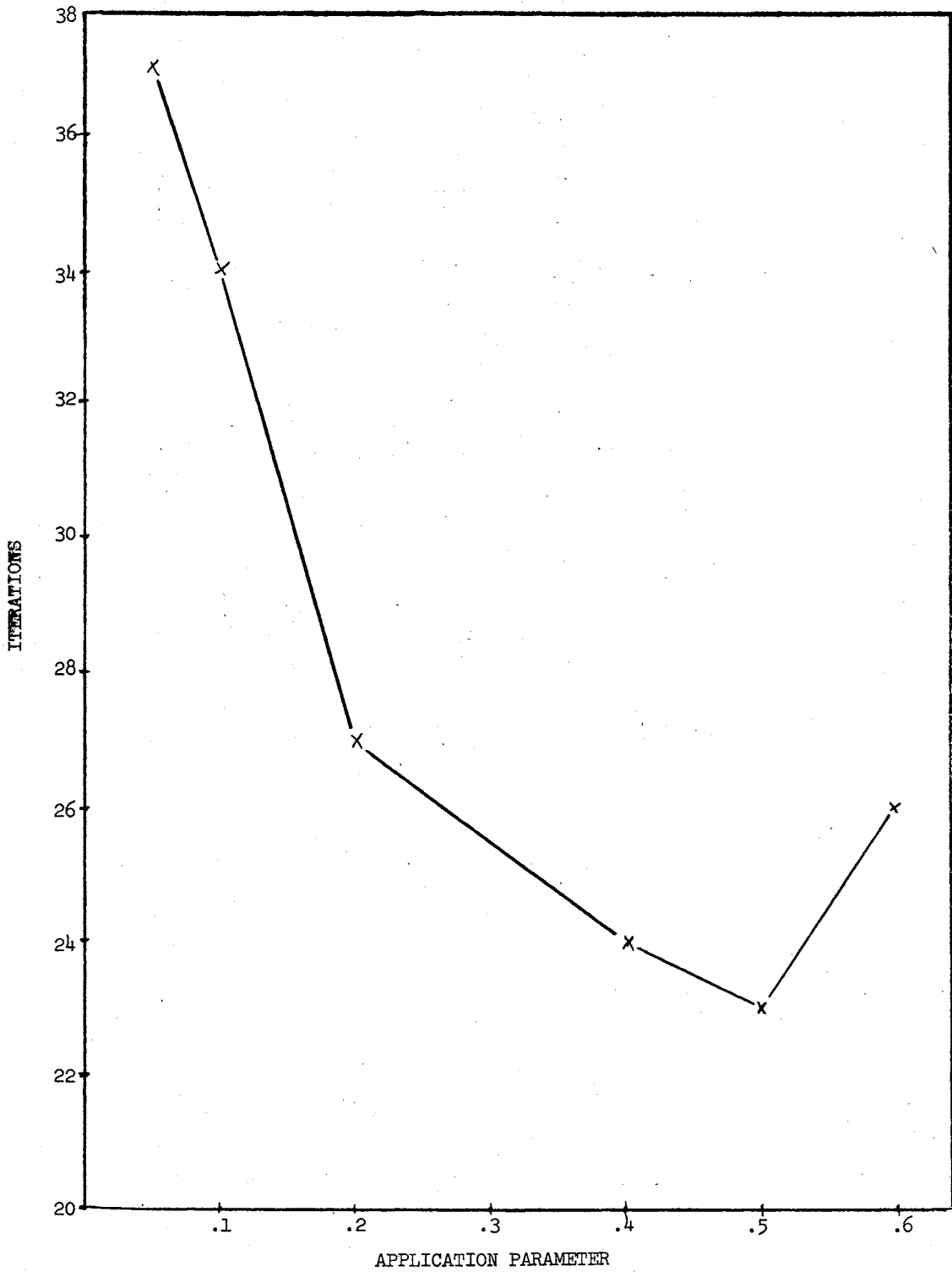
Figure 26.   The Effect of Interaction on the
Application Parameters

Split Fractions

The split fraction method is simply a material balance that deter-
mines the split of each component module and then calculates the
correct feed for the modules corresponding to the specified split and
the raw feed. The main drawback to the method is the limitation of
one feed to each module (unless some extra material balance is
internally applied). If a large migration of the split fraction exists,
a large error is generated between the real and calculated material
balances. The programming involves in the split fraction formulation
is difficult and generalization is complex. Further, the split fraction
formulation is not readily adaptable for reactors since conservation
of molecular species is violated. Even in Problem 7 where the split
fraction technique is carefully constructed for application to this
specific problem, the resulting time ratio of 1.30 as compared with the
Bounded Wegstein (as used with the application parameter) is not
favorable. The split fraction formulation is also tested with the
Bounded Wegstein acceleration technique applied to the split fractions
after three iterations. This method obtains the best time ratio of 0.71
with respect to the Bounded Wegstein using an application parameter of
.2. However, due to the limited range of application of the split
fraction method as constructed, no further effort is made to adapt the
program. Other problems are examined, but no improvement in iteration
count is observed in any case.

Additionally, in Problem 7, the split fraction method exhibits
oscillatory behavior about the solution point. This difficulty is
partially relieved by discontinuing the acceleration procedure when

the value of the total molar flow rate began to diminish as shown in Figure 27.

Among the positive factors about the split fraction technique is the bounded nature of the split fraction variables. Since the split fractions vary between zero and one, the procedure seems quite stable as attested to by the monotonic closure of the iterations. Further, even when the Bounded Wegstein without the application parameter is applied, the closure remained monotonic.

The problems encountered with split fractions are the complexity of programming, the time needed for the matrix inversion, the additional core storage requirement as demanded by the inversion procedure, and the non-applicability of the standard procedure to reactors. Along with these considerations the requirement of additional material balances for multiple feed units and the nonapplicability to energy recycles preclude widespread use of the method.

Algorithm Summary

The Bounded Wegstein (as modified) demonstrates the broadest range of usage in the test cases as evidenced in Table 1 and Figures 27 and 28. When coupled with the simplicity of usage and small time demands, the Bounded Wegstein with a few simple constraints provides the most universally applicable method. The fact remains that the Bounded Wegstein does not always significantly decrease the number of iterations. As the amount of variable interaction increases, the Bounded Wegstein becomes worse in its ability to improve the closure rate. Other methods are somewhat in between successive substitutions and the Bounded Wegstein in effectiveness. The restriction on using
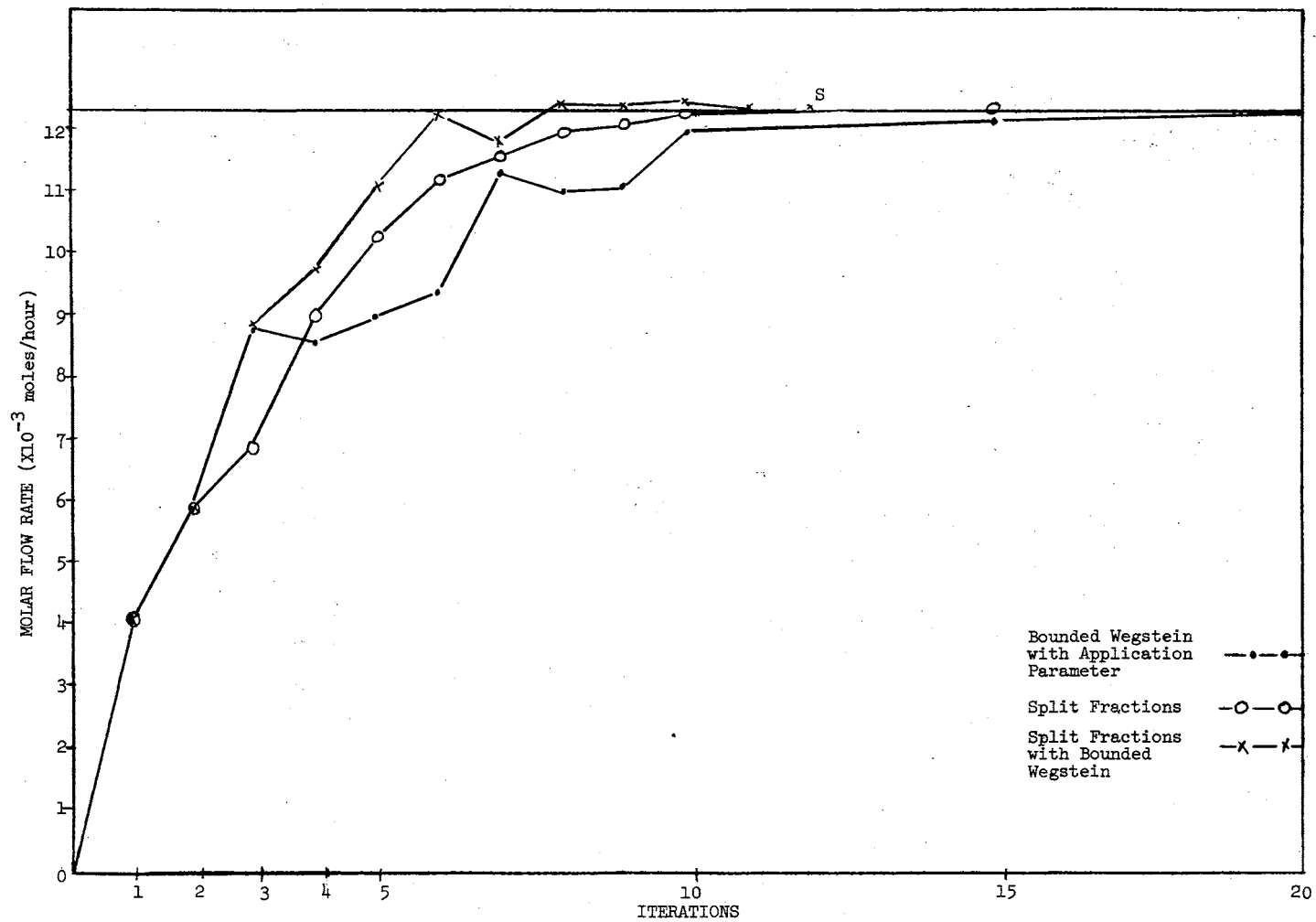
Figure 27. Closure for Stream 9 (Problem No. 7)
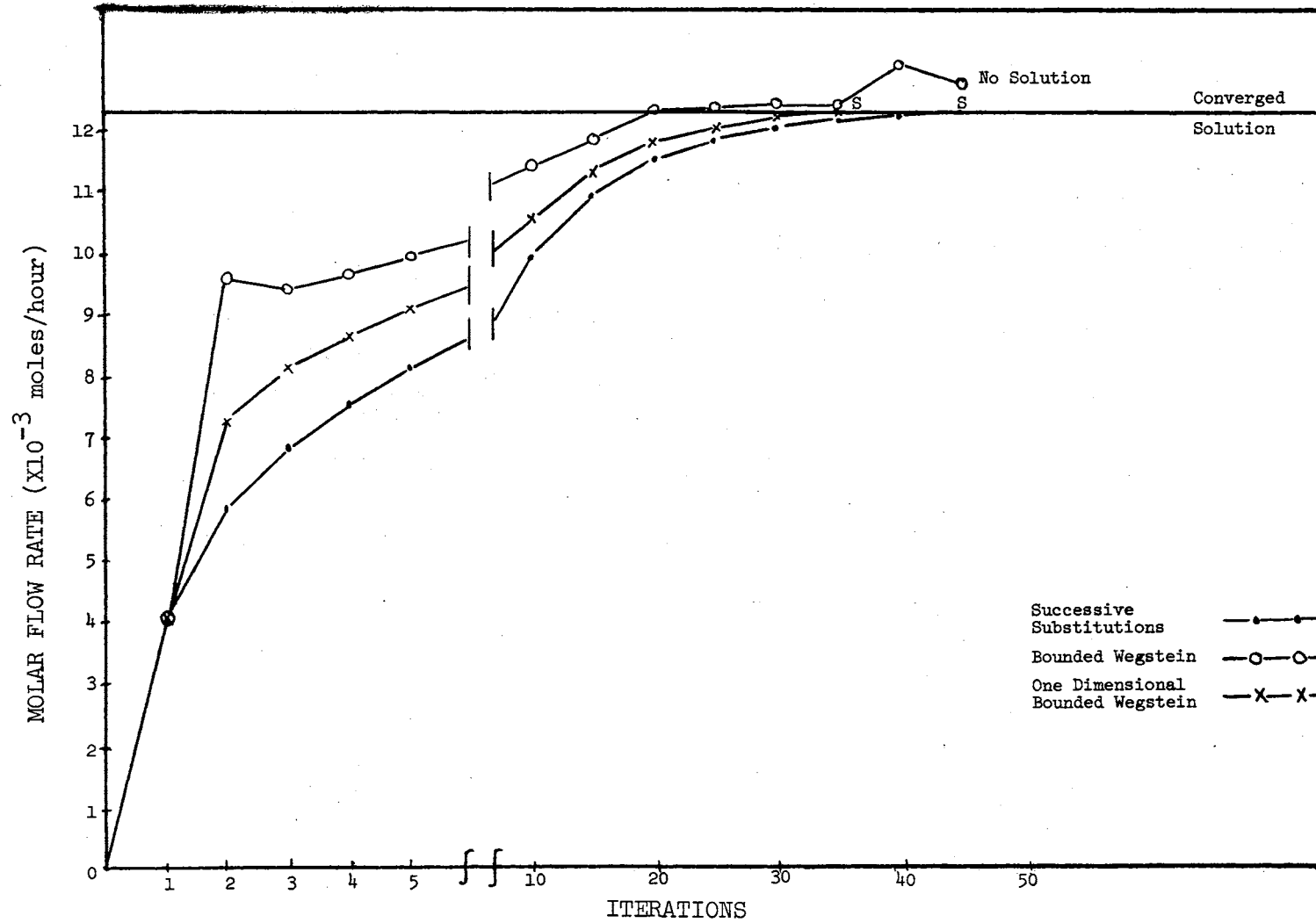
Figure 28. Closure for Stream 5 (Problem No. 7)

a method is the amount of variable interaction in a given problem. In the case of no interaction, all acceleration procedures are satisfactory and some are exact. However, as interaction increases the effect of each acceleration method deteriorates to oscillatory behavior which in some cases inhibits convergence. With the aid of the application bound developed by Orbach and Crowe (12), a flexible parameter is provided for the application of the Bounded Wegstein acceleration method. The application is demonstrated in Figure 29.

Problems

The results of the problems are summarized in Table XIV, page 65. Complete simulation results are located in the appendix, Tables XVI to XXIX. The problems indicated a range of applicability for the various acceleration methods. Problems 1, 3, 4, 5, 6, 8, 9, and 12 represent direct industrial applications. The remainder are selected to use for comparison with the literature (2 and 7) or to illustrate an extreme case (10, 11, 13, and 14). Various factors are postulated to affect the convergence patterns of the recycle streams. Among the factors are:

1. Relative size of recycle stream.

2. Temperature difference between the recycle stream and the stream which the recycle stream enters.

3. "Interaction" between the variables (molar flow rates).

4. Modular interaction (interacting nonlinearities).

5. Network configuration of recycle streams.

Specific cases are presented for the illustration of such behavior.
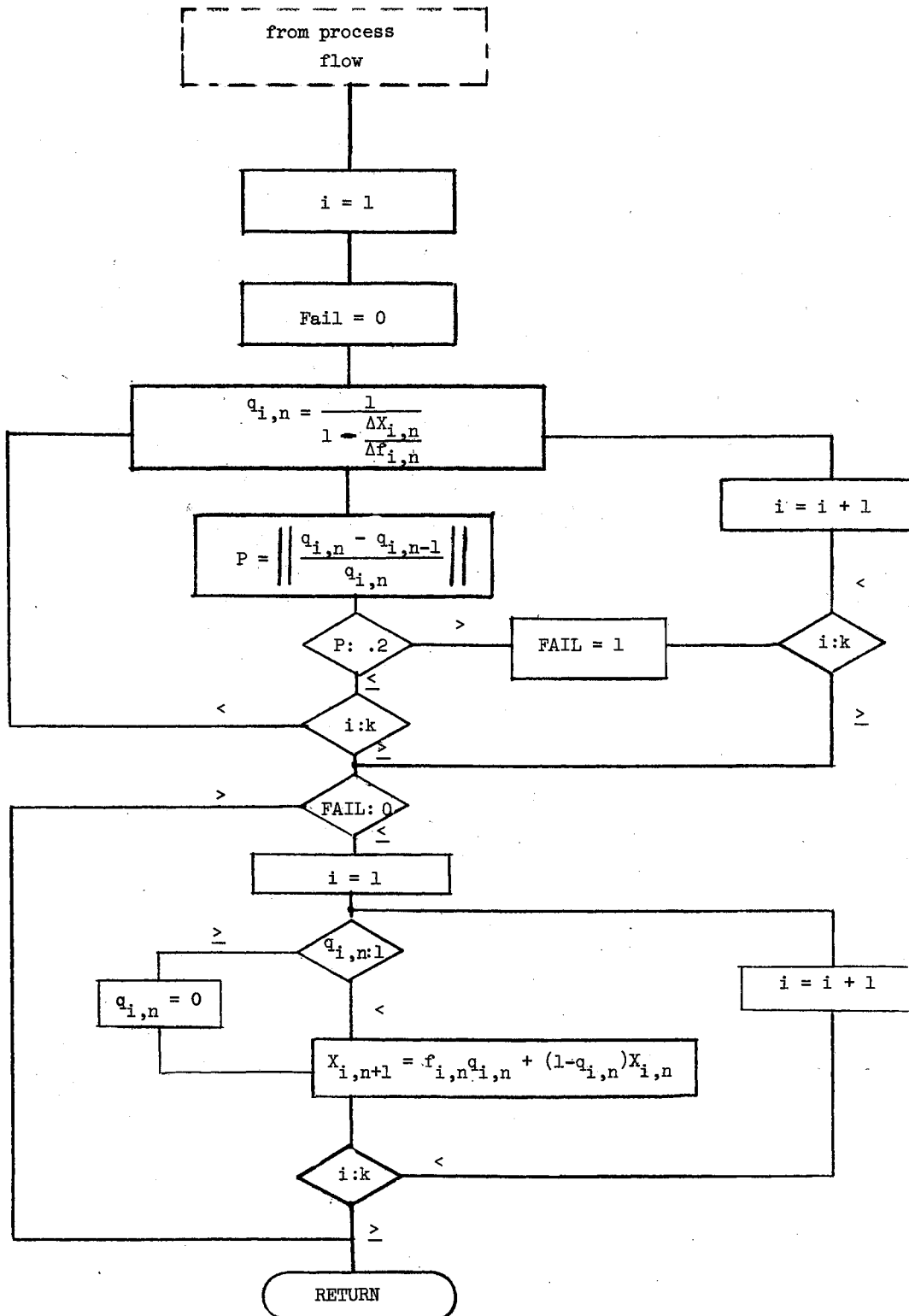
Figure 29. Flow Scheme for Bounded Wegstein with Application Parameter

Problem 1 illustrates a case of an energy recycle alone. No mass is transferred from the recycle stream to the other streams; energy alone, is transferred through the heat exchanger. Although the relative rate of the recycle stream is equivalent to the feed stream and the temperature difference is large, the problem converges quickly. The rapidly converged solution in Problem 1 indicates a relative independence between the temperature of the incoming stream and the split in the first flash unit. Hence, a substantial degree of modular independence is present.

Since the limiting assumption in the Wegstein method is the independence of variables, Problem 11 is created to have no possible interaction. Although large recycle streams are generated by the adder-divider system, the Wegstein method responds by converging the system in a minimal number of iterations. Many permutations of the recycle system have been run and except when round off error becomes significant, the Wegstein performs flawlessly. Strangely enough, however, Problem 12 which also is an adder-divider problem (configuration and overall split is equivalent to Problem 7) is poorly behaved for the convergence accelerators. This problem points toward the network configuration also playing a part in recycle convergence.

Problem 13 is based on a reactor module written specifically for the conversion of toluene to benzene. The goal of the problem is to test the effect of chemical reaction on the convergence schemes. Since the operation of the reactor module is a specified conversion at a given temperature calculating necessary volume, the system becomes as linear and noninteractive as the adder-divider problems and with a single recycle loop responds well to the acceleration algorithms.

Problem 14, although variable interaction is present, demonstrates an intermediate case between the adder-divider system of Problem 11 and Problem 7 which Cavett and Kliesch both examine. The split of the key components is specified in this distillation column representation of Problem 7 (which involved flash units). The time per iteration increases due to the complexity of the distillation calculations. Although the network of the problem is the same as Problem 13 (adder-divider form of Problem 7), the variable interaction as well as the nonlinearity of modular operation slows the convergence time. Nonetheless, the acceleration algorithms are able to affect considerable improvement on the solution. Problem 7 has no specification on the key component split and therefore, permits yet another degree of freedom on the system. Consequently, more iterations are required to solve the problem. But here again significant improvement is noted by the introduction of acceleration techniques. Other intermediate problems are tested using permutations of flash and distillation units, but the results are consistent with the generalizations mentioned as shown in Table XV.

Other problems are presented and the solutions generally adhere to the following rules:

1. The more complex the recycle nesting, the more difficult convergence (even for linear modules) becomes.

2. The larger the amount of recycled material, the more difficult convergence becomes for successive substitutions (this factor does not damage acceleration procedures within the limits of truncation error).

3. The more nonlinear the modular activity, the more the variables "interact," and the more difficult the solution becomes by any procedure.

Obviously, although these observations are true and supported by the
presented problems, no quantitative measure is offered for the pre-
diction of these effects a priori. Variable interaction is measured
as described under the Bounded Wegstein section but could not be
correlated without some knowledge of a quantitative estimate of the
complexity of the recycle nest in the particular problem. Perhaps
this area could be advanced, and the application of the techniques be
made more certain by using an arbitrary application parameter that
seems to work.

TABLE XV

RELATIVE MAGNITUDES OF RECYCLED QUANTITIES

Problem	Iterations	$\frac{R_1}{F_1}$	$\frac{R_2}{F_2}$	$\frac{R_3}{F_3}$	$T_{R1}-T_{F1}$	$T_{R2}-T_{F2}$	$T_{R3}-T_{F3}$
1	7	.94			141.8		
2	24	.44	.655	.937	70.4	70	61.9
3	10	1.0	.027		29.1	10	
4	16	.16	.51		10	133.7	
5	14	1.75	1.45		123	2	
6	8	1.11			2.0		
7	44	.16	.45	.20	20	24	35
8	6	.33			57		
9	6	.40			56		
10	12	1.38	.42		20	63.4	
11	77	8.82	1.0				
12	44	10.8					
13	8	.17	.45	.20			
14	21	.70	.507	.29			

CHAPTER V

RECOMMENDATIONS AND CONCLUSIONS

The problem of recycle convergence is very complex. Among the factors compounding the problem are the nonlinear and ofter iterative procedures used for calculation of most of the various process elements. A network of the process elements represents the process function. The problem is further magnified by the nonlinear nature of the physical properties which are involved with both the element itself and the exit stream properties. On a larger scale the network of elements as well as the magnitude of the material recycled all contribute to the complexity of recycle convergence.

A number of convergence accelerator algorithms are tested in the OSUPAS simulation system using fourteen example problems. The primary methods tested are geometric fitting, the Pourcian, the Bounded Wegstein, and Split Fraction methods. Of all the acceleration methods tested, the Bounded Wegstein performs consistently the best. But the use of an application parameter on the Bounded Wegstein method is required due to undamped oscillation encountered in two cases where the parameter was not employed. With the application parameter, the Bounded Wegstein method represents an improved convergence acceleration algorithm. This improved method, over a large number of cases, provides a saving of money to the user.

Difficulties with the use of the algorithm can be traced to the nonlinear interaction between the molar flow rates. The presence of interaction contradicts the independence assumption. This simplification is necessitated by the magnitude of the analysis followed when interaction is considered. Unfortunately, no way can be presented to evaluate the magnitude of this interaction.

As far as the block-type simulation systems are concerned, little may be done to improve upon acceleration techniques proposed herein. A solution of the simulation problems may be the development of more explicit nonlinear module simulations that are susceptible to the optimization type of analysis. Workers are currently developing a simulation program of this nature. Such efforts are currently regarded as crude and of no direct application in the practical industrial simulation sense but are necessary to evaluate the feasibility of the optimization approach.

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APPENDIX

SIMULATION RESULTS

TABLE XVI

RESULTS FOR COMPRESSOR-EXPANDER (PROBLEM NO. 1)

Stream Number	1	2	3	4	5	6	7	8	9
Methane	5900.00	5900.00	5851.80	5851.80	5817.98	48.20	33.82	5817.98	5817.98
Ethane	410.00	410.00	374.26	374.26	317.83	35.74	56.43	317.83	317.83
Propane	160.00	160.00	102.22	102.22	33.07	57.78	69.15	33.07	33.07
i-Butane	30.00	30.00	10.42	10.42	0.91	19.58	9.51	0.91	0.91
n-Butane	45.00	45.00	10.94	10.94	0.50	34.06	10.44	0.50	0.50
i-Pentane	9.00	9.00	0.88	0.88	0.01	8.12	0.87	0.01	0.01
n-Pentane	15.00	15.00	0.97	0.97	0.01	14.03	0.97	0.01	0.01
n-Heptane	5.00	5.00	0.02	0.02	0.00	4.98	0.02	0.00	0.00
TOTAL	6574.00	6574.00	6351.50	6351.50	6170.29	222.48	181.21	6170.29	6170.29
Temperature, Deg F	95.00	-63.14	-62.95	-136.80	-136.80	-62.95	-136.80	85.00	145.09
Pressure, PSIA	250.00	245.00	245.00	80.00	80.00	245.00	80.00	75.00	98.00
Enthalpy, MMBTU?HR	29.6188	18.4147	19.0672	15.2575	15.9318	-0.6316	-0.6742	27.1330	30.4463
Stream Condition	1.00	0.97	1.00	0.97	1.00	0.00	0.00	1.00	1.00
Molecular Weight	18.35	18.35	17.48	17.48	16.93	43.20	36.33	16.93	16.93
Density LB/CUFT	0.80086	1.21492	1.12056	0.43974	0.41402	32.57431	30.04347	0.21943	0.25796

TABLE XVII

RESULTS FOR CAVETT'S SECOND PROBLEM (PROBLEM NO. 2)

Stream Number	1	2	3	4	5	6	7	8	9
Methane	8276.00	8327.03	8327.03	8327.01	8327.01	8327.01	8200.87	8200.87	8200.87
Ethane	871.00	940.10	940.10	940.10	940.10	940.10	851.28	851.28	851.28
Propane	411.00	556.45	556.45	556.43	556.43	556.43	394.69	394.69	394.69
i-Butane	28.00	50.57	50.57	50.57	50.57	50.57	24.60	24.60	24.60
n-Butane	113.00	225.64	225.64	225.64	225.64	225.64	87.96	87.96	87.96
i-Pentane	25.00	45.02	45.02	45.01	45.01	45.01	9.45	9.45	9.45
n-Pentane	32.00	51.56	51.56	51.51	51.51	51.51	8.18	8.18	8.18
n-Hexane	21.00	23.66	23.66	23.66	23.66	23.66	1.24	1.24	1.24
n-Heptane	12.00	12.32	12.32	12.32	12.32	12.32	0.23	0.23	0.23
Carbon Dioxide	20.00	20.82	20.82	20.82	20.82	20.82	19.58	19.58	19.58
Nitrogen	191.00	191.17	191.17	191.17	191.17	191.17	190.32	190.32	190.32
TOTAL	10000.00	10444.31	10444.31	10444.21	10444.21	10444.21	9788.38	9788.38	9788.38
Temperature, Deg F	70.00	75.56	252.24	61.85	29.59	0.00	0.00	51.85	58.09
Pressure, PSIA	150.00	150.00	400.00	395.00	392.00	390.00	390.00	380.00	370.00
Enthalpy, MMBTU/HR	43.9653	47.3912	66.6940	43.4927	38.2491	32.8333	33.9465	39.1885	39.8810
Stream Condition	1.00	1.00	1.00	1.00	0.97	0.94	1.00	1.00	1.00
Molecular Weight	19.86	20.97	20.97	20.96	20.96	20.96	19.28	19.28	19.28
Density LB/CUFT	0.54055	0.56609	1.13241	1.63771	1.79629	1.99424	1.73307	1.45237	1.38897

TABLE XVII (Continued)

Stream Number	10	11	12	13	14	15	16	17	18
Methane	8276.01	126.17	126.17	75.14	51.03	51.03	0.00	0.00	8327.01
Ethane	870.74	88.75	88.75	19.46	69.30	69.10	0.19	0.19	940.10
Propane	407.33	161.74	161.74	12.64	149.10	145.45	3.65	3.65	556.43
i-Butane	25.51	25.97	25.97	0.91	25.06	22.57	2.49	2.49	50.57
n-Butane	91.48	137.68	137.68	3.52	134.16	112.64	21.53	21.53	225.64
i-Pentane	9.86	35.57	35.57	0.41	35.16	20.02	15.13	15.13	45.01
n-Pentane	8.56	43.39	43.39	0.38	43.00	19.56	23.45	23.45	51.51
n-Hexane	1.31	22.42	22.42	0.07	22.36	2.66	19.69	19.69	23.66
n-Heptane	0.25	12.09	12.09	0.01	12.08	0.32	11.75	11.75	12.32
Carbon Dioxide	20.00	1.23	1.23	0.42	0.82	0.82	0.00	0.00	20.82
Nitrogen	191.00	0.85	0.85	0.68	0.17	0.17	0.00	0.00	191.17
TOTAL	9902.01	655.87	655.87	113.64	542.23	444.33	97.90	97.90	10444.21
Temperature, Deg F.	52.95	0.00	60.00	54.18	54.18	144.39	237.03	52.85	70.00
Pressure, PSIA	300.00	390.00	380.00	300.00	300.00	150.00	150.00	140.00	398.00
Enthalpy, MMBTU/HR	40.3662	-1.1135	0.0512	0.4879	-0.4367	3.4265	0.5458	-0.1466	44.6584
Stream Condition	1.00	0.00	0.13	1.00	0.00	1.00	0.00	0.00	1.00
Molecular Weight	19.33	46.13	46.13	23.82	50.81	45.75	73.77	73.77	20.96
Density LB/CUFT	1.12621	33.24492	15.68814	1.44709	33.99922	1.20959	37.98782	39.45732	1.61464

TABLE XVIII

RESULTS FOR OLEFIN TANK REFRIGERATION SYSTEM (PROBLEM NO. 3)

Stream Number	1	2	3	4	5	6	7	8
Propane	192.50	204.18	11.68	192.48	11.68	11.68	11.68	11.68
i-Butane	452.50	464.50	12.00	452.48	12.00	12.00	12.00	12.00
n-Butane	515.00	525.24	10.24	514.99	10.24	10.24	10.24	10.24
i-Pentane	505.00	509.53	4.53	504.99	4.53	4.53	4.53	4.53
Propylene	400.00	428.15	28.15	399.95	28.15	28.15	28.15	28.15
i-Butene	532.50	544.52	12.02	532.48	12.02	12.02	12.02	12.02
i-Pentene	267.50	269.65	2.15	267.50	2.15	2.15	2.15	2.15
TOTAL	2865.00	2946.78	80.78	2864.87	80.78	80.78	80.78	80.78
Temperature, Deg F	105.00	105.29	115.06	100.91	100.91	120.00	215.19	130.00
Pressure, PSIA	200.00	200.00	257.00	75.00	75.00	74.00	260.00	259.00
Enthalpy, MMBTU/HR	-0.2264	-0.2142	0.0122	-0.7976	0.5833	0.6167	0.7435	0.0456
Stream Condition	0.00	0.00	0.00	0.00	1.00	1.00	1.00	0.00
Molecular Weight	58.16	57.97	51.31	58.16	51.31	51.31	51.31	51.31
Density LB/CUFT	36.26096	36.21339	34.45183	36.20245	0.70469	0.66502	2.32078	34.32265

TABLE XIX

RESULTS FOR RECOMPRESSION PLANT (PROBLEM NO. 4)

Stream Number	1	2	3	4	5	6	7	8
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.10	0.10	0.00
Carbon Dioxide	0.10	0.10	0.00	0.10	0.10	0.90	1.07	0.00
Methane	5.10	5.19	0.01	5.19	5.19	73.40	80.19	0.09
Ethane	5.80	5.95	0.03	5.93	5.93	20.10	28.86	0.15
Propane	10.40	10.90	0.17	10.73	10.73	14.70	28.81	0.50
i-Butane	4.60	5.09	0.19	4.90	4.90	4.70	12.13	0.49
n-Butane	4.40	4.90	0.24	4.74	4.74	3.40	10.97	0.58
i-Pentane	1.80	2.43	0.26	2.17	2.17	1.10	5.44	0.63
n-Pentane	1.20	1.74	0.23	1.51	1.51	0.60	3.82	0.54
n-Heptane	1.80	4.38	2.39	1.99	1.99	0.80	4.58	2.58
n-Nonane	0.00	0.18	0.16	0.02	0.02	0.00	0.19	0.18
TOTAL	35.20	40.95	3.68	37.27	37.27	119.80	176.15	5.75
Temperature, Deg F	110.00	100.44	110.00	110.00	188.69	100.00	92.20	100.00
Pressure, PSIA	30.00	30.00	30.00	30.00	90.00	90.00	90.00	90.00
Enthalpy, MMBTU/HR	0.2625	0.2635	0.0020	0.2817	0.3389	0.6295	0.9523	0.0010
Stream Condition	1.00	0.89	0.00	1.00	1.00	1.00	0.96	0.00
Molecular Weight	46.57	51.17	89.38	47.40	47.40	26.26	33.88	79.32
Density LB/CUFT	0.23503	0.29669	41.08318	0.23944	0.65266	0.40492	0.56159	39.66931

TABLE XIX (Continued)

Stream Number	9	10	11	12	13	14	15
Nitrogen	0.10	0.10	0.33	0.43	0.00	0.43	0.43
Carbon Dioxide	1.07	1.07	2.93	4.00	0.07	3.93	3.93
Methane	80.10	80.10	185.33	265.43	1.60	263.82	263.82
Ethane	28.71	28.71	62.28	90.99	2.83	88.15	88.15
Propane	28.31	28.31	6.33	34.64	3.38	31.26	31.26
i-Butane	11.64	11.64	0.75	12.39	2.53	9.86	9.86
n-Butane	10.38	10.38	0.38	10.76	2.83	7.94	7.94
i-Pentane	4.81	4.81	0.04	4.85	2.17	2.68	2.68
n-Pentane	3.27	3.27	0.02	3.29	1.70	1.59	1.59
n-Heptane	2.00	2.00	0.00	2.00	1.79	0.21	0.21
n-Nonane	0.02	0.02	0.16	0.18	0.18	0.00	0.00
TOTAL	170.40	170.40	258.55	428.95	19.08	409.87	409.87
Temperature, Deg F	100.00	214.43	55.00	135.02	55.00	55.00	224.77
Pressure, PSIA	90.00	280.00	280.00	280.00	280.00	280.00	1025.00
Stream Condition	1.00	1.00	1.00	1.00	0.00	1.00	1.00
Molecular Weight	32.35	32.35	20.71	25.33	55.32	23.94	23.94
Density LB/CUFT	0.50643	1.35451	1.13119	1.19195	35.03120	1.34439	3.80979

TABLE XX

RESULTS FOR ABSORBER NETWORK (PROBLEM NO. 5)

Stream Number	10	11	12	13	14	15	16
Hydrogen	0.00	2013.64	1971.90	41.70	41.70	65.33	65.33
Hydrogen Sulfide	2.20	4.30	2.18	2.12	2.12	0.06	0.06
Methane	0.00	346.83	306.98	39.82	39.82	37.26	37.26
Ethane	0.00	279.23	177.14	102.05	102.05	64.46	64.46
Propane	0.00	172.17	63.64	108.45	108.45	136.33	136.33
i-Butane	0.00	9.89	2.04	7.86	7.86	33.82	33.82
n-Butane	2.20	12.02	1.97	10.05	10.05	45.93	45.93
Hypothetical Component 1	1629.40	1695.56	6.24	1689.41	1689.41	1632.61	0.00
Hypothetical Component 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL	1633.80	4533.64	2532.08	2001.46	2001.46	2015.80	383.19
Temperature, Deg F	110.00	156.64	110.00	110.00	233.00	226.87	226.87
Pressure PSIA	544.00	544.00	544.00	544.00	544.00	624.00	624.00
Enthalpy, MMBTU/HR	3.9651	20.7543	10.5564	4.6868	16.2642	15.7737	2.8631
Stream Condition	0.00	0.57	1.00	0.00	0.00	0.00	1.00
Molecular Weight	111.92	47.89	7.12	99.46	99.46	97.40	34.75
Density, LB/CUFT	46.83661	6.01347	0.62691	45.27165	44.52390	44.50763	3.63289

TABLE XX (Continued)

Stream Number	17	18	19	20	21	22	23
Hydrogen	0.00	1994.50	2059.83	2037.28	22.55	2037.28	2013.64
Hydrogen Sulfide	0.00	0.00	0.06	0.04	0.02	0.04	2.10
Methane	0.00	330.50	367.76	344.27	23.49	344.27	346.83
Ethane	0.00	249.70	314.16	241.63	72.53	241.63	279.23
Propane	0.00	248.70	385.03	199.94	185.08	199.94	172.17
i-Butane	0.00	78.60	112.42	35.87	76.55	35.87	9.89
n-Butane	0.00	129.00	174.93	45.69	129.24	45.69	9.82
Hypothetical Component 1	1632.61	1412.50	1412.50	9.35	1403.15	9.35	66.16
Hypothetical Component 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL	1632.61	4443.50	4826.69	2914.08	1912.60	2914.08	2899.84
Temperature, Deg F	226.87	110.00	121.29	110.00	110.00	231.00	233.00
Pressure, PSIA	624.00	324.00	324.00	324.00	324.00	324.00	620.00
Enthalpy, MMBTU/HR	14.0911	15.3826	18.2456	12.9403	3.8742	16.3007	16.7891
Stream Condition	0.00	0.60	0.61	1.00	0.00	1.00	1.00
Molecular Weight	112.10	44.61	43.82	10.81	94.12	10.81	11.81
Density, LB/CUFT	46.33899	3.64787	3.49042	0.57440	44.07520	0.47111	0.97971

TABLE XXI

RESULTS FOR GAS CLEANUP BEFORE DEPROPANIZER (PROBLEM NO. 6)

Stream Number	1	2	3	4	5	6	7	8	9
Methane	50.30	61.05	61.02	49.65	0.00	38.91	10.75	10.75	11.36
Ethane	78.40	131.22	131.21	64.33	0.00	11.51	52.82	52.82	66.88
Propane	120.60	156.10	156.22	35.68	0.00	0.18	35.50	35.50	120.54
i-Butane	172.60	194.48	194.55	21.88	0.00	0.01	21.88	21.88	172.67
n-Butane	243.70	266.81	266.88	23.11	0.00	0.00	23.11	23.11	243.77
i-Pentane	5.10	5.31	5.31	0.21	0.00	0.00	0.21	0.21	5.10
n-Pentane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Lean Oil	0.00	600.69	600.69	0.69	600.00	0.00	600.69	600.69	600.00
TOTAL	670.70	1415.66	1415.88	195.56	600.00	50.60	744.96	744.96	1220.32
Temperature, Deg F	120.00	156.83	100.00	100.00	100.00	100.00	123.03	122.03	100.00
Pressure, PSIA	111.00	95.00	90.00	90.00	80.00	90.00	80.00	95.00	90.00
Enthalpy, MMBTU/HR	5.0596	8.5690	3.8472	1.1807	2.6275	0.2362	3.5719	3.5093	2.6665
Stream Conditon	0.99	0.29	0.14	1.00	0.00	1.00	0.00	0.00	0.00
Molecular Weight	49.27	82.71	82.71	35.92	130.00	19.34	112.82	112.82	90.21
Density LB/CUFT	1.00855	7.76495	7.76495	0.56956	43.56520	0.29434	41.97598	41.98514	40.06017

TABLE XXII

RESULTS FOR CAVETT'S FIRST PROBLEM (PROBLEM NO. 7)

Stream Number	1	2	3	4	5	6
Nitrogen	358.20	400.48	22.40	378.06	19.88	358.18
Carbon Dioxide	4965.60	7939.34	1895.57	6042.46	1082.85	4959.61
Hydrogen Sulfide	339.40	783.18	326.37	456.65	122.71	333.95
Methane	2995.50	3780.64	466.11	3314.15	319.10	2995.05
Ethane	2395.50	4885.40	1724.52	3159.90	780.44	2379.46
Propane	2291.00	7930.11	4812.45	3115.68	1236.11	1879.57
i-Butane	604.10	1731.87	1326.64	404.92	209.05	195.87
n-Butane	1539.90	3673.39	2973.44	699.50	400.90	298.60
i-Pentane	790.40	1166.64	1048.63	117.98	80.30	37.68
n-Pentane	1129.90	1535.67	1407.71	127.95	92.55	35.39
n-Hexane	1764.70	1954.86	1888.58	66.29	55.59	10.70
n-Heptane	2606.70	2711.54	2671.66	39.89	36.09	3.80
n-Octane	1844.50	1871.61	1860.45	11.16	10.60	0.56
n-Nonane	1669.00	1678.80	1674.47	4.33	4.21	0.12
n-Decane	831.70	833.79	832.80	0.98	0.97	0.02
n-Undecane	1214.50	1215.87	1215.19	0.69	0.68	0.01
TOTAL	27340.59	44093.16	26146.96	17940.56	4451.99	13488.54
Temperature, Deg F	120.00	79.48	120.00	120.00	100.00	100.00
Pressure, PSIA	270.00	49.00	270.00	270.00	800.00	800.00
Enthalpy, MMBTU/HR	70.1148	152.1759	29.0870	93.5708	1.5630	50.0229
Stream Conditon	0.34	0.64	0.00	1.00	0.00	1.00
Molecular Weight	68.48	59.72	75.03	37.42	43.54	35.41
Density LB/CUFT	8.04567	0.80137	39.54614	1.83061	35.07968	7.50530

TABLE XXII (Continued)

Stream Number	7	8	9	10	11
Nitrogen	22.63	0.23	22.40	0.00	0.23
Carbon Dioxide	2029.76	139.00	1890.89	4.87	134.18
Hydrogen Sulfide	381.10	59.99	321.07	5.28	54.73
Methane	479.60	13.66	466.04	0.18	13.49
Ethane	1946.26	236.53	1709.47	14.83	221.74
Propane	6481.77	2074.89	4403.00	404.49	1669.33
i-Butane	1978.27	1058.24	918.72	405.66	651.63
n-Butane	4424.73	2689.83	1732.59	1236.56	1451.29
i-Pentane	1398.19	1101.94	295.94	752.05	349.56
n-Pentane	1801.22	1487.69	313.22	1093.83	393.51
n-Hexane	2082.58	1947.89	134.57	1753.77	194.00
n-Heptane	2771.90	2703.08	68.75	2602.80	100.24
n-Octane	1883.78	1867.25	16.52	1843.91	23.33
n-Nonane	1682.03	1676.43	5.59	1668.87	7.56
n-Decane	834.25	833.13	1.12	831.68	1.45
n-Undecane	1216.04	1215.35	0.69	1214.49	0.86
TOTAL	31414.10	19105.13	12300.56	13833.26	5267.11
Temperature, Deg F	45.62	96.00	96.00	85.00	85.00
Pressure, PSIA	13.00	49.00	49.00	13.00	13.00
Enthalpy, MMBTU/HR	70.8625	5.9659	80.4980	-0.1674	41.7745
Stream Condition	0.51	0.00	1.00	0.00	1.00
Molecular Weight	71.83	88.40	46.12	100.76	55.98
Density LB/CUFT	0.34330	40.98279	0.39602	42.49292	0.12692

TABLE XXIII

RESULTS FOR ABSORBER (PROBLEM NO. 8)

Stream Number	1	2	3	4	5	6	7
Hydrogen	63.40	0.00	63.40	63.40	0.00	0.00	0.00
Methane	119.60	0.00	127.96	119.60	8.36	8.36	0.00
Ethane	134.80	0.00	186.67	134.77	51.90	51.87	0.03
Propane	90.56	0.00	184.17	35.27	148.90	51.87	55.29
i-Butane	11.30	0.00	11.57	0.05	11.52	0.27	11.25
n-Butane	29.60	0.00	29.94	0.02	29.92	0.34	29.58
n-Pentane	3.70	0.00	3.72	0.00	3.72	0.02	3.70
Hydrogen Sulfide	2.20	0.00	3.33	2.19	1.14	1.13	0.01
Hypothetical Component x	9.30	0.00	9.32	0.00	9.32	0.02	9.30
Hypothetical Component 1	0.00	25.76	0.03	1.23	24.56	0.03	24.53
Hypothetical Component 2	0.00	51.44	0.03	1.29	50.18	0.03	50.15
Hypothetical Component 3	0.00	77.10	0.03	0.00	77.13	0.03	77.10
Hypothetical Component 4	0.00	102.81	0.03	0.00	102.84	0.03	102.81
Hypothetical Component 5	0.00	257.02	0.05	0.00	257.07	0.05	257.02
Hypothetical Component 6	0.00	154.24	0.02	0.00	154.26	0.02	154.24
Hypothetical Component 7	0.00	102.87	0.00	0.00	102.88	0.01	102.87
TOTAL	469.16	771.24	624.97	357.81	1038.39	155.81	882.58
Temperature, Deg F	100.00	100.00	83.65	115.00	133.56	43.30	294.80
Pressure, PSIA	100.00	100.00	100.00	96.00	98.00	100.00	100.00
Enthalpy, MMBTU/HR	2.6558	1.7799	3.4366	1.8343	3.3821	0.7810	10.8502
Stream Condition	1.00	0.00	1.00	1.00	0.00	1.00	0.00
Molecular Weight	29.62	116.43	31.71	22.28	97.88	37.99	108.45
Density LB/CUFT	0.51384	46.46425	0.57344	0.35386	43.65807	0.78465	43.97685

TABLE XXIV

RESULTS FOR ABSORBER (PROBLEM NO. 9)

Stream Number	1	2	3	4	5	6	7
Hydrogen	63.40	0.00	63.40	63.40	0.00	0.00	0.00
Methane	119.60	0.00	130.09	119.60	10.49	10.49	0.00
Ethane	134.80	0.00	204.64	134.75	69.89	69.84	0.05
Propane	90.56	0.00	193.02	19.29	173.73	102.46	71.26
i-Butane	11.30	0.00	11.62	0.02	11.60	0.32	11.28
n-Butane	29.60	0.00	30.07	0.01	30.07	0.47	29.59
i-Pentane	3.70	0.00	3.72	0.00	3.72	0.02	3.70
n-Pentane	4.70	0.00	4.72	0.00	4.72	0.02	4.70
Hydrogen Sulfide	2.20	0.00	3.47	2.19	1.28	1.27	0.01
Hypothetical Component x	9.30	0.00	9.32	0.00	9.32	0.02	9.30
Hypothetical Component 1	0.00	30.74	0.05	1.15	29.64	0.05	29.59
Hypothetical Component 2	0.00	61.39	0.05	0.00	61.44	0.05	61.39
Hypothetical Component 3	0.00	92.01	0.06	0.06	92.07	0.06	92.01
Hypothetical Component 4	0.00	122.70	0.05	0.00	122.75	0.05	122.70
Hypothetical Component 5	0.00	306.73	0.09	0.00	306.82	0.09	306.73
Hypothetical Component 6	0.00	184.07	0.03	0.00	184.10	0.03	184.07
Hypothetical Component 7	0.00	122.77	0.01	0.00	122.78	0.01	122.77
TOTAL	469.16	920.42	654.41	340.40	1234.43	185.26	1049.17
Temperature, Deg F	100.00	100.00	81.98	115.00	132.41	44.42	293.17
Pressure, PSIA	100.00	100.00	100.00	96.00	98.00	100.00	100.00
Enthalpy, MMBTU/HR	2.5557	2.1241	3.5800	1.7027	4.0013	0.9245	12.7983
Stream Condition	1.00	0.00	1.00	1.00	0.00	1.00	0.00
Molecular Weight	29.62	116.43	31.80	20.95	97.90	37.34	108.59
Density LB/CUFT	0.51384	46.46425	0.57760	0.33189	43.65855	0.76637	44.00972

TABLE XXV

RESULTS FOR COMPLETE STRIPPER-ABSORBER SYSTEM (PROBLEM NO. 10)

Stream Number	1	2	3	4	5
Methane	50.30	61.06	61.07	55.00	50.30
Ethane	78.40	193.40	193.42	129.17	78.40
Propane	120.60	498.88	499.05	191.64	20.51
i-Butane	172.60	220.86	220.87	46.82	0.37
n-Butane	243.70	293.11	293.09	49.13	0.14
i-Pentane	5.10	5.56	5.56	0.46	0.00
n-Pentane	0.00	0.00	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00
Lean Oil	0.00	598.98	598.98	1.51	2.67
TOTAL	670.70	1871.84	1872.02	473.72	152.39
Temperature, Deg F	120.00	142.50	100.00	100.00	100.00
Pressure, PSIA	111.00	80.00	75.00	90.00	90.00
Enthalpy, MMBTU/HR	5.0596	11.3630	6.5273	2.9922	0.8314
Stream Condition	0.99	0.47	0.32	1.00	1.00
Molecular Weight	49.27	73.16	73.15	40.16	29.17
Density LB/CUFT	1.00855	1.96609	2.83656	0.64699	0.45368

TABLE XXV (Continued)

Stream Number	6	7	8	9	10
Methane	6.06	0.00	6.06	0.00	4.70
Ethane	64.25	0.02	64.23	0.00	50.77
Propane	307.41	100.25	207.15	0.00	171.13
i-Butane	174.05	172.24	1.82	0.00	46.45
n-Butane	243.95	243.54	0.42	0.00	48.99
i-Pentane	5.10	5.10	0.00	0.00	0.46
n-Pentane	0.00	0.00	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00
Lean Oil	597.47	597.34	0.13	600.00	598.84
TOTAL	1398.29	1118.48	279.81	600.00	921.33
Temperature, Deg F	100.00	185.76	56.62	100.00	140.01
Pressure, PSIA	90.00	95.00	95.00	80.00	80.00
Enthalpy, MMBTU/HR	2.6114	7.1835	1.5157	2.6275	4.7886
Stream Condition	0.00	0.00	1.00	0.00	0.00
Molecular Weight	84.33	95.32	40.42	130.00	100.48
Density, LB/CUFT	39.32448	40.11765	0.76922	43.56520	40.72920

TABLE XXVI

RESULTS FOR ADDER-DIVIDER (PROBLEM NO. 11)

Stream Number	1	2	3	4	5	6	7
Nitrogen	358.20	3519.89	7932.86	3512.98	351.30	3512.98	3161.69
Carbon Dioxide	4965.60	48794.91	97494.06	48699.23	4869.92	48699.21	43829.31
Hydrogen Sulfide	339.40	335.15	663.75	3328.61	332.86	3328.60	2995.75
Methane	2995.50	29435.68	58813.63	29377.97	2937.80	29377.96	26440.18
Ethane	2395.50	23539.69	47033.23	23493.55	2349.35	23493.54	21144.19
Propane	2291.00	22512.81	44981.47	22468.68	2246.87	22468.66	20221.81
i-Butane	604.10	5936.23	11860.82	5924.59	592.46	5924.59	5332.13
n-Butane	1539.90	15132.01	30234.34	15102.35	1510.23	15102.33	13592.11
i-Pentane	790.40	7766.95	15518.66	7751.72	775.17	7751.71	6976.55
n-Pentane	1129.90	11103.09	22184.41	11081.32	1108.13	11081.32	9973.19
n-Hexane	1764.70	17341.04	34648.07	17307.05	1730.70	17307.03	15576.34
n-Heptane	2606.70	25615.07	51179.91	25564.86	2556.48	25564.85	23008.37
n-Octane	1844.50	18125.22	36214.89	18089.69	1808.97	18089.67	16280.72
n-Nonane	1669.00	16400.64	32769.12	16368.49	1636.85	16368.48	14731.64
n-Decane	831.70	8172.79	16329.55	8156.77	815.68	8156.76	7341.09
n-Undecane	1214.50	11934.43	23845.46	11911.04	1191.10	11911.03	10719.93
TOTAL	27340.59	268665.25	536803.81	268138.44	26813.87	268138.31	241324.63
Temperature, Deg F	120.00	120.00	120.00	120.00	120.00	120.00	120.00
Pressure, PSIA	270.00	270.00	270.00	270.00	270.00	270.00	270.00
Enthalpy, MMBTU/HR	70.1148	689.0088	1376.6907	687.6703	68.7670	687.6697	618.9028
Stream Condition	0.34	0.34	0.34	0.34	0.34	0.34	0.34
Molecular Weight	68.48	68.48	68.48	68.48	68.48	68.48	68.48
Density LB/Cuft	8.04567	8.04560	8.04558	8.04561	8.04558	8.04559	8.04561

TABLE XXVII

RESULTS FOR BENZENE REACTOR WITH RECYCLE (PROBLEM NO. 12)

Stream Number	1	2	3	4	5
Hydrogen	0.00	156.81	146.71	146.59	146.46
Toluene	20.00	20.20	10.10	10.10	0.22
Benzene	0.00	0.61	10.71	10.71	0.68
Methane	0.00	83.66	93.76	93.67	92.95
TOTAL	20.00	261.28	261.28	261.07	240.31
Temperature, Deg F	500.30	1300.30	1312.07	70.00	70.00
Pressure, PSIA	500.00	500.00	500.00	500.00	500.00
Enthalpy, MMBTU/HR	0.2217	4.9542	4.9546	0.7777	0.9168
Stream Condition	0.00	0.94	1.00	0.92	1.00
Molecular Weight	92.13	13.65	13.65	13.66	7.74
Density, LB/CUFT	51.16753	0.35828	0.35599	1.28530	0.67824

TABLE XXVII (Continued)

Stream Number	6	7	8	9
Hydrogen	0.13	14.65	25.00	131.81
Toluene	9.88	0.02	0.00	0.20
Benzene	10.03	0.07	0.00	0.61
Methane	0.72	9.30	0.00	83.66
TOTAL	20.76	24.03	25.00	216.28
Temperature, Deg F	70.00	70.00	70.00	70.00
Pressure, PSIA	500.00	500.00	500.00	500.00
Enthalpy, MMBTU/HR	-0.1391	0.0917	0.0902	0.8252
Stream Condition	0.00	1.00	1.00	1.00
Molecular Weight	82.16	7.74	2.02	7.74
Density, LB/CUFT	53.95784	0.67824	0.17366	0.67824

TABLE XXVIII

RESULTS FOR ADDER-DIVIDER FORM OF CAVETT'S FIRST PROBLEM (PROBLEM NO. 13)

Stream Number	1	2	3	4	5	6
Nitrogen	358.20	579.71	343.37	413.09	250.75	181.04
Carbon Dioxide	4965.60	8036.25	2760.05	5726.51	3475.99	2509.67
Hydrogen Sulfide	339.40	549.28	325.35	391.41	237.58	171.54
Methane	2995.50	4847.88	2871.50	3454.53	2096.90	1513.96
Ethane	2395.50	3876.85	2296.34	2762.58	1676.89	1210.71
Propane	2291.00	3707.73	2196.17	2642.07	1603.74	1157.90
i-Butane	604.10	977.67	579.09	696.67	422.88	305.32
n-Butane	1539.90	2492.16	1476.16	1775.87	1077.96	778.28
i-Pentane	790.40	1279.17	757.68	911.52	553.29	399.48
n-Pentane	1129.90	1828.62	1083.13	1303.04	790.95	571.06
n-Hexane	1764.70	2855.97	1691.65	2035.12	1235.32	891.90
n-Heptane	2606.70	4218.65	2498.80	3006.15	1824.73	1317.46
n-Octane	1844.50	2985.12	1768.15	2127.15	1291.18	932.23
n-Nonane	1669.00	2701.09	1599.91	1924.76	1168.33	843.53
n-Decane	831.70	1346.01	797.27	959.15	582.20	420.35
n-Undecane	1214.50	1965.53	1164.23	1400.61	850.17	613.82
TOTAL	27340.59	44247.65	26208.82	31530.20	19138.83	13818.23
Temperature, Deg F	120.00	120.00	120.00	120.00	120.00	120.00
Pressure, PSIA	270.00	270.00	270.00	270.00	270.00	270.00
Enthalpy, MMBTU/HR	70.1148	113.4758	67.2142	80.8625	49.0836	35.4383
Stream Condition	0.34	0.34	0.34	0.34	0.34	0.34
Molecular Weight	68.48	68.48	68.48	68.48	68.48	68.48
Density,LB/CUFT	8.04567	8.04558	8.04558	8.04559	8.04560	8.04560

TABLE XXVIII (Continued)

Stream Number	7	8	9	10	11
Nitrogen	236.65	59.16	117.49	162.34	69.71
Carbon Dioxide	3280.58	820.14	2460.43	2250.52	966.33
Hydrogen Sulfide	224.23	56.06	168.17	153.82	66.05
Methane	1979.01	494.75	1484.26	1357.63	582.94
Ethane	1582.61	395.65	1186.96	1085.69	466.18
Propane	1513.58	378.39	1135.18	1038.33	445.84
i-Butane	399.11	99.78	299.33	273.79	117.56
n-Butane	1017.35	254.34	763.01	697.92	299.67
i-Pentane	522.19	130.55	391.64	358.23	153.82
n-Pentane	746.48	186.62	559.86	512.10	219.88
n-Hexane	1165.87	291.47	874.40	799.80	343.42
n-Heptane	1722.14	430.54	1291.61	1181.41	507.28
n-Octane	1218.59	304.65	913.94	835.97	358.95
n-Nonane	1102.64	275.66	826.98	756.43	324.79
n-Decane	549.47	137.37	412.10	376.94	161.85
n-Undecane	802.37	200.59	601.78	550.44	236.35
TOTAL	18062.84	4515.71	13547.13	12391.35	5320.59
Temperature, Deg F	120.00	120.00	120.00	120.00	120.00
Pressure, PSIA	270.00	270.00	270.00	270.00	270.00
Enthalpy, MMBTU/HR	46.3233	11.5808	34.7425	31.7789	13.6452
Stream Condition	0.34	0.34	0.34	0.34	0.34
Molecular Weight	68.48	68.48	68.48	68.48	68.48
Density, LB/CUFT	8.04559	8.04557	8.04560	8.04560	8.04557

TABLE XXIX

RESULTS FOR CAVETT'S FIRST PROBLEM (DIST) (PROBLEM NO. 14)

Stream Number	1	2	3	4	5	6
Nitrogen	358.20	400.68	22.64	378.04	19.84	358.20
Carbon Dioxide	4965.60	7940.13	1901.46	6038.67	1077.81	4960.86
Hydrogen Sulfide	339.40	782.60	326.38	456.22	122.11	334.11
Methane	2995.50	3782.72	469.45	3313.27	318.08	2995.19
Ethane	2395.50	4882.77	1725.36	3157.41	776.86	2380.55
Propane	2291.00	7894.84	4786.64	3108.21	1228.54	1879.67
i-Butane	604.10	1732.71	1325.63	407.07	209.46	197.61
n-Butane	1539.90	3677.66	2973.14	704.51	402.51	302.01
i-Pentane	790.40	1168.53	1049.27	119.26	80.97	38.29
n-Pentane	1129.90	1538.17	1408.70	129.48	93.44	36.03
n-Hexane	1764.70	1956.86	1889.52	67.33	56.38	10.95
n-Heptane	2606.70	2713.02	2672.37	40.65	36.74	3.91
n-Octane	1844.50	1872.09	1860.68	11.41	10.83	0.58
n-Nonane	1669.00	1679.01	1674.57	4.44	4.32	0.13
n-Decane	831.70	833.84	832.83	1.01	1.00	0.02
n-Undecane	1214.50	1215.91	1215.20	0.71	0.70	0.01
TOTAL	27340.59	44071.51	26133.82	17937.68	4439.57	13498.08
Temperature, Deg F	120.00	79.63	119.66	120.77	100.26	100.40
Pressure, PSIA	270.00	49.00	270.00	270.00	800.00	800.00
Enthalpy, MMBTU/HR	70.1148	152.2525	28.7639	93.7980	1.5875	50.1694
Stream Condition	0.34	0.64	0.00	1.00	0.00	1.00
Molecular Weight	68.48	49.74	75.04	37.44	43.59	35.42
Density, LB/CUFT	8.04567	0.80144	39.55499	1.82845	35.09039	7.49449

TABLE XXIX (Continued)

Stream Number	7	8	9	10	11
Nitrogen	22.88	0.24	22.64	0.00	0.24
Carbon Dioxide	2036.94	140.31	1896.63	4.95	135.36
Hydrogen Sulfide	381.32	60.25	321.07	4.34	54.91
Methane	483.15	13.89	469.26	0.18	13.70
Ethane	1948.13	237.74	1710.39	15.00	222.73
Propane	6443.97	2065.38	4378.59	404.59	1660.79
i-Butane	1976.10	1056.98	919.11	406.53	650.45
n-Butane	4422.14	2686.98	1735.16	1238.47	1448.51
i-Pentane	1398.13	1100.97	297.16	752.12	348.85
n-Pentane	1801.55	1486.71	314.83	1093.86	392.85
n-Hexane	2083.54	1947.77	135.77	1753.75	194.01
n-Heptane	2772.76	2703.19	69.58	2602.78	100.40
n-Octane	1884.09	1867.32	16.76	1843.92	23.41
n-Nonane	1682.16	1676.47	5.69	1668.87	7.60
n-Decane	834.28	833.14	1.14	831.68	1.45
n-Undecane	1216.07	1215.36	0.71	1214.49	0.86
TOTAL	31387.18	19092.66	12294.51	13836.54	5256.11
Temperature, Deg F	45.53	95.84	96.45	84.89	85.16
Pressure, PSIA	13.00	49.00	49.00	13.00	13.00
Enthalpy, MMBTU/HR	70.4644	5.8484	80.5677	-0.2366	41.7084
Stream Condition	0.51	0.00	1.00	0.00	1.00
Molecular Weight	71.86	88.42	46.13	100.75	55.99
Density, LB/CUFT	0.34403	40.98779	0.39576	42.49269	0.12689

VITA

Toby Robert Graves

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Doctor of Philosophy

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PROCESS RECYCLE CALCULATIONS

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