SYNTHESIS OF SEPARATION SCHEMES

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July 1972

ABSTRACT

The ability of the computer to synthesize complex separation schemes has been investigated and demonstrated. Several new concepts were generated as a result of the evolving programming study. The hierarchical ordering of executive routines in a synthesis system allows great flexibility in adding or modifying detailed simulation routines for separator units. Products rather than components are being separated; this concept is important when there are multicomponent products. A Product Separability Matrix was created to identify the candidate separations and to eliminate those which are infeasible as early as possible in the selection process. Incorporation of heuristics into the programming was done where no algorithmic procedure could be ascertained or where the use of heuristic procedures would save time without a major loss of generality. A number of heuristics were designed and evaluated.

A new general heuristic which should be of value to the design engineer, whether or not he is using the computer, is that the next separator to be incorporated into the separator sequence at any point is the one that is cheapest. This rule-of-thumb is useful when the candidate feasible separator sequences have been identified previously, as with the Product Separability Matrix. This heuristic rule has been

explored in some depth, and factors leading to exceptions from the rule have been identified.

A number of illustrative examples are included.

1. INTRODUCTION

The design of a chemical production process can roughly be divided into two steps--synthesis and analysis. Extensive attention has been given to analysis, but very little study has been devoted to the synthesis phase or process design, i.e., the creation of the process scheme. Synthesis problems involve inductive as well as deductive logic, and are not single-answered. They are open-ended, and hence more qualitative--e.g., one can never be sure that one has considered all candidate separation processes, or all possible feeds from which something could be made. Synthesis and analysis generally deal with different types of variables. Analysis of a specified process (for the purpose of optimization, say) involves the use of continuous variables, e.g., temperature, pressure, flow rate, and mole fractions--variables that are differentiable and that are susceptible to handling by familiar mathematical techniques. Synthesis, on the other hand, cannot at present be approached in such a rigorous manner as analysis because it deals with discrete variables, which can take on only certain values, generally 0 and 1. Considering for example a separation system, either a certain separator is in the process or it is not--there are no other possibilities.

A chemical production process generally consists of a reaction section followed by a section for chemical isolation (or separation). Often more than two products are to be produced in the separation section. This will involve the use of more than one separation unit (separator), and not only the choice of the type of separator but also the sequence of the units is important. The work of this dissertation is concerned with the synthesis step of the process design of a separation scheme.

As an indication of the number of different sequences of units which are possible and may merit attention, consider the example of the sequencing of single-feed, two-product separators which are all the same type of separation unit (e.g., distillation). For simplicity, this separation unit is chosen to be one which does not require a mass separating agent (i.e., a solvent or an absorption or extraction agent). The number of possible sequences for separation of N components from each other into single-component products is given by the following closed-form equation (see Appendix A):

$$\text{Number of sequences} = \frac{(2(N-1))!}{N! (N-1)!} \quad (1)$$

For $N = 4$, Fig. 1 illustrates a complete enumeration of the alternative sequences. For seven components the number of different sequences possible is 132.

Usually more than one type of separation unit is considered, however. A different type of separator is one that has a different configuration of stages, or derives its separation ability from a different principle, or uses a different mass separating agent which can affect the separability of the chemical components present. If S different separator types are to be considered at each constituent step in the sequence, the number of different sequences (not considering recovery of mass separating agents used) increases from the number given in Eq. (1) by a factor of S^{N-1} , since each of the $N-1$ separators in each scheme could be replaced by one of the S candidate units. For the seven-product scheme, considering ten candidate units increases the number of schemes to $132 \times (10)^{7-1} = 132$

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Fig. 1. The five possible arrangements of three separators.

million. It is understandably infeasible to examine individually all of the possible schemes, even with a computer.

Previous Work

Previous studies have reported on the sequencing of distillation units. Lockhart (1947) studied several existing distillation sequences and made specific recommendations but drew no conclusions of general applicability to other systems. Harbert (1957) considered sequencing from the point of view of optimizing only the heating requirements. Rod and Marek (1959) also considered the sequencing problem in general, with more examples, and a very detailed costing of the distillation units (Heaven, 1970). Maikov and Abramov (1965) approach the sequencing as a dynamic programming problem, rewriting equations describing component distributions to fit that format. Nishimura and Hiraizumi (1971) considered distillation sequencing in a very mathematical manner but must assume either that all of the components are in about the same concentration or that one dominates. Heuristics for synthesis, largely drawn from the examples furnished by Heaven, appear in Separation Processes (King, 1971).

Rough, qualitative work has been done on comparison between distillation, extractive distillation, and extraction for a single separation task (Souders, 1964). This was based on assumed solvent concentrations and liquid flow rates, and the conclusions related needed separation factors for equal plant costs for the different processes. Simultaneous with the dissertation work presented here, Hendry and Hughes (1972) considered more than one type of separator in synthesizing a separation train. They used the approach of dynamic programming, as

did Maikov and Abramov (1965) for distillation. Their approach is to assume perfect separation and to begin at the end of the process calculating all binary separations that are possible, all possible ternary separators, etc. This is done for a variety of feed conditions since the upstream conditions have not yet been established. The cheapest combination is chosen to make the process. Because of its close relation to this work, more discussion of the Hendry and Hughes work is included in Chapter 7.

Other pioneering work in synthesis of chemical processes, though not specifically separation trains, has been done. Heat exchange networks have been synthesized by weighting heuristics (Masso, 1968), by a branch-and-bound method (Masso, et al., 1970), and by linear programming (Kesler and Parker, 1969). Synthesis of the entire chemical plant by centering on the chemical reactors has been studied by Siirola and later by Powers (see Siirola and Rudd, 1971).

Problem Statement

The problem that is attacked in this dissertation is: Given a feed stream of known conditions (i.e., composition, flow rate, temperature, and pressure), systematically synthesize a process that can isolate specified products from the feed at minimum cost.

$$\min \left(\sum_i c_i \right) \quad i \in I$$

and I is an ordered subset of S , each element $i \in I$ is feasible to build and operate as a separation unit

and S is the set of all possible separator and component-split combinations

subject to I being able to produce feasibly the specified products from the feed stream.

A variety of separator types are to be considered. The input information is to be kept to a minimum. No chemical reactors are to be considered in the same process, but any solvents used are to be recycled.

Definitions

Some of the terms used in this dissertation are uncommon or used with special meaning. Split fraction is the fraction of the feed quantity of a component that is recovered in the produce in which that component appears most predominantly. Key components for a separation are the two components on whose split fractions the separator is designed. The key components are taken as the two components to separate, i.e., the pair of components, one of which appears predominantly in each product of a separator, which have a separation factor closest to unity. A separation factor between two components is the ratio of the two distribution coefficients of those two components. The distribution coefficient is based on the ratio of component mole fraction in the lighter state to that in the heavier state of aggregation at equilibrium, or, if that does not apply, in solvent phase to feed phase. Key products are the two products passing through a separator containing the key components. The light key component is the component having the greater distribution coefficient; the other is the heavy key component. A mass separating agent is a component that is

added to a separation unit to affect the desired separation. This is contrasted to an energy separating agent, wherein energy is used to affect the separation. When both are used, e.g., extractive distillation, the separation unit is characterized as a mass-separating-agent separator. An algorithm is taken as a mathematical procedure which is guaranteed to accomplish the given task. On the other hand, a heuristic is defined as a rule-of-thumb method which often reaches the desired goal, but cannot be shown to always do so.

2. GENERAL STRATEGY

Choice of Strategy

Synthesis of separation trains involves calculations of high complexity. No way could be found to formulate the problem as a tractable objective function which could be solved as an optimization problem, in the normal sense. Furthermore, the character of the problem is such that there is no way to confirm optimality without almost an exhaustive search.

In one conceivable approach the problem could be considered as a large graph having several levels of nodes, each level representing the possible choices of separators to be used at that point in the train. The problem could then be stated as finding the cheapest path from the first level to the last. Each node in the graph would represent a separator-type and component-split combination. A cost could be associated with each of these nodes (or of the arc leading to it). Unfortunately, the cost of a separation unit depends on the value of a number of variables that lead to it, and in general would depend on all of the separators that preceded it (i.e., the path that it took to get to that node). Since each node cost depends on the path to arrive at it, to assign a single cost to a node there must be a single path to the node. The graph is thus a tree, with no cross-linking; each node has only one path directed toward it. The number of nodes is very large. Many of the costs of the nodes are quite competitive; thus a cheapest-path algorithm may be close to the exhaustive search mentioned in Chapter 1, and described by Eq. (1).

If it is assumed, on the other hand, that the cost of each separator (node) is independent of the other separators (nodes) preceding it in the path, the problem of a cheapest path is much smaller: there are only

$S(N)(N+1)/2$ nodes in the graph. (S and N being as defined in Chapter 1.) But this assumption of independence is very unrealistic. The strategy used in this dissertation (as well as the approaches of the other workers mentioned below) is to seek some middle ground. The goal of this research is to find a procedure which can find a path or some paths through the graph which satisfies the problem statement but does not require excessive computation time. This method will be based in part on heuristics and cannot be guaranteed to be optimal. It will account for some, but not all, of the dependence of the cost of a separator on the path used in reaching that point in the process.

Some of the workers mentioned in Chapter 1 have attempted to approach problems of synthesis as just an optimization problem. For separators, costing of the units could not be linearized to use the successive linear programming approach of Kesler and Parker, nor is the costing simple and fast enough to use the branch-and-bound technique of Masso and Rudd (1969). Dynamic programming (Hendry and Hughes, 1972) can be used only after accepting simplifying assumptions about distribution coefficients, upstream conditions, and mass separating agents that are unrealistic in an attack on the general problem of separation scheme synthesis.

As is the case with the methods mentioned above, algorithmic procedures were sought to solve, if not the entire problem, then parts of the problem. Filling the gaps between the algorithms that were developed in this work, heuristics were used on various decision levels. The heuristics used do not represent the only way that the problem could

be attacked, and the successes and short-comings of these heuristics are discussed at length in this dissertation.

Computer Programming

The computer was used as a vehicle to force a logical approach to the synthesis problem, as well as to demonstrate the success of the synthesis procedures developed. The work represented here is not intended as a specific computer program for immediate use in creating separation trains; however, the research can best be described by explaining how the computerized synthesizer functions. The computer provides for full documentation and subsequent assessment of the logic used in systematizing the process synthesis. The programming has been done exclusively in FORTRAN for ease of understanding by other workers, for compatibility between machines, and for more efficient coding of arithmetic operations (compared to list-processing languages). All programs described here appear in the appendices of this dissertation. The state of progress toward efficient and general systematic synthesis logic can be evaluated by testing the ability of the programmed logic to succeed in a variety of problem situations. The logic can then be altered or extended in ways suggested by the types of failures and inadequacies which are encountered.

Decision Making

The basic approach taken to the synthesis problem involves evaluation and decision-making without having the logic encumbered by large amounts of specific information that is not essential to the decisions at hand. In terms of computer programming this means organizing

the decision processes on several levels, using several executive routines, each of which in ascending hierarchy has less and less information available to it about the particulars of the chemical separation process to be synthesized. Hence, decisions are made with as little information as possible while having those decisions be broadly applicable to as many specific situations as possible. Information flows are required to transmit the decisions downward and feed the results of those decisions upward for evaluation. The original problem is transformed with the computer into Boolean-type matrices, in order to provide information for clear-cut choices.

General Procedure

Focussing on the separations problem more specifically, the general procedure of the synthesis is described below. Although a separation unit separates components, a separation train, seen as a whole, creates products. Some or all of the desired products may be groups of components, rather than individual chemical species. Desired multicomponent products may not always be feasible to produce without splitting the components and subsequently remixing. Thus the first task is to decide what the products are that a separation train can feasibly produce. Strong preference is given here, as a heuristic, to using a set of products that has the least number of splits of the desired products. This preference may not lead to the best process, and the application of this heuristic at this point may subsequently be negated by evolutionary changes in the feasible product set.

The product set selection, as well as elimination of some unusable candidate separations, is handled in the computer program by routine PROD

(see Fig. 2). Information on all of the feasible candidate separators is manipulated and transmitted from PROD by a three-dimensional matrix called the Product Separability Matrix.

Once products have been established and all usable candidate separations have been identified, a process flowsheet which will given these products is synthesized under the direction of routine SYNT. SYNT handles the bookkeeping concerning the distribution of products in effluent streams, but is not concerned with the particular chemical components present, excepting the keys. SYNT shares some of the synthesis procedure with PICK, a routine which selects the next separation to be made at any point in the sequence. The selection of separators starts with the feed and proceeds in the direction of material flow. This direction allows calculation of input information for successor units; the quantities of all components, including monkey%, in the feed to each unit are always known. Such a complete feed description is not available with calculations in the reverse direction, such as used in the dynamic programming approach of Hendry and Hughes (1972).

After the flowsheet is created, routine DETAIL takes over the sizing and costing of the process. It calls on simulation routines for the separation units that are needed, and handles the interchange of information between units. The detailed costing of the unit is relayed back to SYNT to be used in the re-evaluation of the predicted cost of the unit. This information is used by PICK in further unit selection. A new flowsheet is then produced, sized, and costed. This procedure is repeated until SYNT cannot find a better (lower-cost) process. At this juncture yet another heuristic, favoring energy-separating-agents over mass-separating-agents, is tested. Separation units on the flowsheet which are not energy-

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Fig. 2. General strategy.

separating-agent processes are examined to see if their presence is necessitated by the requirement of a multicomponent product. If this is so, PROD splits the product so that the energy-separating-agent process can be considered in its stead. SYNT then reworks the flowsheet in the manner described above.

Detailed Description

Chapter 3 discusses the creation of the product set, the workings of routine PROD, and the Product Separability Matrix. The flowsheet synthesis and the associated routines are described in Chapter 4. Chapter 5 describes the detailed simulations of the process and units. Sample problems that were run on the computer synthesizer are discussed in Chapter 6.

3. FEASIBLE PRODUCT SET

Routine PROD transforms information on the desired products and distribution coefficients into information for direct use by the synthesizer SYNT) in decision-making. The routine has effectively six entry points, listed and described as follows:

- (0) Initial creation of feasible product sets.
- (1) Elimination of a potential product set or product separations.
- (2) Activation of a new product set.
- (3) Activation of potential product separations.
- (4) Multicomponent product splitting.
- (5) Elimination of a product set created by (4).

Initial Creation of Product Set

For a process in which the desired products are all single components, the feasible product set is just a list of all the feed components as individual products. In that case this section of PROD is trivial. However, if one or more of the desired products is multicomponent, i.e., two or more components wanted or allowed to be in the same product, the feasibility of producing this multicomponent product must be determined. If several such products are possible but all are not simultaneously possible, decisions must be made concerning which will be incorporated into the product set that will be selected for the synthesizer.

From the distribution coefficients for the components, the components are ordered for each type of separation process in the order of decreasing separation factor. The distribution coefficients are given initial estimates for this purpose, by computing them at a standard temperature and pressure (130°F and 14.7 psia, respectively) and for a solution composition equal to the feed composition. Components in any given desired product are

combined into all possible pairs. The positions of the paired components in the order of decreasing distribution coefficients for each candidate separation process are then examined. If any one other component divides the pair in the orderings for all the separators, that pair cannot feasibly be isolated as part of a single product. All pairs that are found to be feasible to produce are listed and numbered. A three-dimensional Pair Compatability Matrix is created, indexing the pairs against themselves and also against the types of separation units. This matrix is Boolean, having non-zero elements a_{ijk} whenever pair i can be separated from pair j by separator k . ($a_{ijk} = a_{jik}$.) The Pair Compatability Matrix is then examined to create feasible production sets of pairs that are found to be mutually separable. (Mutual separability exists if each pair can be separated from all other pairs.) These feasible production sets are ordered by decreasing number of included pairs, and duplicates are eliminated. Within each of the product sets thus created, pairs having components in common are combined into single-product subsets. These subsets plus all feasible pairs which are in the production set, plus all other components in the feed not already listed are incorporated as separate products in the product set. All of the available mass-separating-agents specified in the input information are also added to the product set as potential single-component products. The product set with the greatest number of pairs, i.e., the least number of feed-component separations, is now alone considered in subsequent process synthesis operations. This invokes the heuristic that the best process will have the least number of feed-component products. If more than one product set appears attractive, the other sets may be considered later. This decision can later be altered

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Fig. 3. Product Separability Matrix.

either by activating a new product set or by splitting a multicomponent product in the existing set.

Product Separability Matrix

With the above-selected product set a highly-utilized, three-dimensional matrix is created. This Product Separability Matrix conveys to all the executive routines information on the following points:

1. Feasibility of separation between any two products by any given separation unit.
2. Presence of products in the stream to be separated.
3. Separation adjacency of any two products (i.e., whether they would be the key products in a separation).
4. Names of the components that could be light and heavy keys in a separation.
5. Which of any two products that can be separated has the larger distribution coefficient.

Reduction of Problem Size

Because of the presence of multicomponent products, not all of the product pairs which are separable individually can be separated from the mixture without splitting a multicomponent product. Such infeasible separations are eliminated in the Product Separability Matrix (Entry 2).

This point is rather subtle and is best understood by considering the following example: Given three products: 1,2,3, having components 5,6,7,8 distributed among them as follows,

Product Number

1
2
3

Component Number

7
8
5,6

The separation ordering for the components in the three available types of separators are

Separator Number	<u>1</u>	<u>2</u>	<u>3</u>
	5	5	5
	7	7	8
	8	6	6
	6	3	7

The Product Separability Matrix has element a_{ij} of value -1 if and only if product i can be separated from product j by separator k and product j has larger distribution coefficients than product i . The matrix would initially appear as this:

Separator Number <u>1</u>				<u>2</u>				<u>3</u>			
$j = 1 \quad 2 \quad 3$				$j = 1 \quad 2 \quad 3$				$j = 1 \quad 2 \quad 3$			
$i = 1$	0	0	0	$i = 1$	0	0	0	$i = 1$	0	-1	-1
2	-1	0	0	2	-1	0	-1	2	0	0	0
3	0	0	0	3	0	0	0	3	0	0	0

Any -1 entry in this matrix is a potential separation to be considered. However, for Separator Number 1 the indicated separation is infeasible, not because a 1/2 product split there would split product 3, but because there exists no scheme which could remove product 3 (without splitting it) before the 1/2 separation is made. This fact is evidenced by there being no separator which has -1 entries for both $a_{2,3,k}$ and $a_{1,3,k}$, or for both $a_{3,2,k}$ and $a_{3,1,k}$. Thus the $a_{2,1,1}$ value must be returned to zero. This is an instance of another basic concept used in this work, namely, that infeasible solutions are identified and eliminated from consideration as soon as possible.

The algorithm that was developed for accomplishing the task described in the above example is as follows:

Product i can be separated from Product j by Separator s if and only if a non-zero value appears in the Product Separability Matrix at

- A. One of the two: (i,j,s)
 (j,i,s)

and

B. For all multicomponent products MP, except i and j :

1. One of the four: (MP,i,s)
 (MP,j,s)
 (i,MP,s)
 (j,MP,s)

or

2. For some separator x :

- a. (MP,j,x) and (MP,i,x)

or

- b. (j,MP,x) and (i,MP,x)

All potential products (not components) appear as indices in the Product Separability Matrix, whether or not they are in the mixture to be separated. This matrix is used by other executive routines, such as SYNT and PICK--routines which need to know which of the potential products are actually present in the mixture which is to be separated by some means. This information is transmitted through the Product Separability Matrix by altering to positive numbers the values of the non-zero entries which correspond to products that are present in the mixture (stream) under consideration and are potential key products for the separation. This alteration (Entry 3) also codes into the matrix the names of the potential heavy and light key components. Referring to the previous example, suppose that

the same three products were present and contained the same components.

The altered matrix would look like this:

Separator Number <u>1</u>				<u>2</u>				<u>3</u>			
j = 1 2 3				j = 1 2 3				j = 1 2 3			
i = 1	0	0	0	i = 1	0	0	0	i = 1	0	-1	706
2	0	0	0	2	-1	0	806	2	0	0	0
3	0	0	0	3	0	0	0	3	0	0	0

The 806 indicates to the routines that Product 2 can be separated from Product No. 3 by Separator No. 2, and that the light key in such a separation is component 6 and the heavy key is component 8. Similar meaning applies to the 706. Only those two candidate separations can and need to be considered in choosing a separation to be made on this mixture. The other two -1 values remain unchanged because, although they are potential separations, they cannot be made at this point in the sequence. Product No. 3 is present in the mixture, and would be split by either of the two separations for which the -1 values are left unaltered.

Not only does this procedure reduce the scope as soon as possible in the synthesis procedure and thereby reduce the information to be handled, but it also ensures that PICK has just exactly the right field of choice each time--namely, those candidate next-separation processes which can feasibly lead to the given product set.

If the 706 separation is now chosen, the result will be two mixtures--one containing Product No. 1, and the other containing Products 2 and 3. At this point PROD is again called to alter the Product Separability Matrix so that it will apply to the mixture of Products 2 and 3. The altered matrix now looks like this:

Separator Number 1

	j = 1	2	3
i = 1	0	0	0
2	0	0	0
3	0	0	0

2

	j = 1	2	3
i = 1	0	0	0
2	-1	0	806
3	0	0	0

3

	j = 1	2	3
i = 1	0	-1	-1
2	0	0	0
3	0	0	0

The entries relating to Product 1 remain at -1 since Product 1 is not present. Again, only the positive entries are to be considered in choosing a separation, so the 806 separation will necessarily be chosen. The following diagram shows the resulting process:

Alteration of the Product Set

Feasible product sets, once created, can be changed by having a multicomponent product split into two products (Entry 4). Such a change is suggested whenever the stabilized process contains one (or more) separators which require the use of a mass-separating-agent and when it is not possible for an energy-separating-agent separator to be used to split the same two keys. Such a situation can only arise if at least one of the keys is a multicomponent product. The incentive for such a heuristic change is

the need for an extra separator to recover the mass-separating-agent at at some later point in the process. The existence of this extra separator was not considered in choosing the original product set. This heuristic could be called: "Why not distillation?".

The two key products of such a separator are considered for splitting in creating the new product set. One or the other is divided so as to make an energy separation unit a candidate for the future separation of the components in the products. The split is made in a way that will minimize the number of new products that are created. If one of the two new products is not multicomponent, there is only one place to split the other product. If both are multicomponent, two places are considered for the split, namely, at the points in the distribution coefficient ranking that define the extremities of the other new product. For example, if A identifies components in one product and B in the other, the split points would be as below:

```
A
A _____ could split A's here
B
B
A
B
A _____ could split B's here
B
B
```

Only one can be selected for the new product set; the others are added to the list of potential product sets. If the use of this split product set is not found to result in an overall lower-cost process, it is eliminated by calling for Entry 5, which restores the old product set.

4. FLOWSHEET SYNTHESIS

Once the feasible product set has been established, the pertinent information is passed to the synthesis routines via the Product Separability Matrix. The actual synthesis is guided by routine SYNT, but the feasible choices of key products and separator at any given point in the process are presented by the Product Separability Matrix. Decisions on those choices are made by routine PICK, based on heuristics. The synthesizing sequence follows the natural flow of material through the process. On each stream, beginning with the initial feed, SYNT lists the products that are present (by number) and calls on PROD (through Entry 3) to alter the Product Separability Matrix so as to define the key products and components for that stream, as described in Chapter 3. PICK then uses the list of products present in the stream, the Product Separability Matrix, the distribution coefficients (calculated at the standard conditions), and estimates of separator costs to decide which is the best separation to be made on that stream.

SYNT accepts the decisions of PICK and uses the Product Separability Matrix to distribute all of the products present (again, by number) between the two effluent streams of the chosen separator. This distribution is simple to accomplish, because the Product Separability Matrix, by indexing all of the products against themselves, indicates for any separator which products are "lighter" than another product by having a non-zero entry in the matrix. If the particular separation chosen requires the use of a mass-separating-agent, SYNT will also denote the agent's presence in the appropriate effluent stream. This mass-separating-agent becomes then another product to be separated from all other products for recycle at some yet

undesigned point in the process. Each of the effluent streams is assigned to a stream number, and information about the products present, the type of separator chosen to effect a separation upon it (i.e., a separator which uses the stream as a feed stream), as well as key products and key components is recorded. The routine SYNT then works sequentially on the effluent streams in exactly the same manner, until all final streams contain only one product.

So as to link all of the streams together, the eventual information recorded about any stream that is the feed to a separator includes the number of the effluent "light" or "overhead" stream. (For this purpose, the "overhead" stream in liquid-liquid extraction is always not the feed phase.) The number of the other effluent stream is then one greater than the number of the overhead stream. If a mass-separating-agent is used, the number of the stream where it has been isolated as a single product is indicated for recycle purposes. The split fraction of the mass-separating-agent is arbitrarily set as 0.995.

Separator Selection

Decision power for choosing the separator type and the key components is concentrated in routine PICK. Centering of the heuristic decision rules in one routine allows for each changes in the rules. All feasible combinations of separators and key components (i.e., all items with positive entries in the current Product Separability Matrix) are considered in applying these rules each time PICK is called to make a choice. The number of combinations is not as great as it may seem at first since

the Product Separability Matrix allows that only feasible combinations need be considered.

As implemented in this work, the governing heuristic is based on economics and the updating of economic factors, based on detailed simulating of the processes, through estimated cost-weighting factors. This use of weighting factors for costs is not to be confused with weighting factors on heuristics, which were not used. The general heuristic which was used in nearly all of the present work for choosing a separator and its keys is that the best separator is the one from among those feasible that is cheapest to add at that point in the process. This is a generalization of several more limited heuristics (King, 1971):

- (1) Leave high recovery fractions until last.
- (2) Leave separators with small separation factors until last.
- (3) Have the pressure decreasing through the train.
- (4) Make a 50/50 split in each separator.

Limited Heuristics No. 1 and No. 2 fall naturally into the general heuristic of "cheapest first". Both high recovery fractions and small separation factors make for expensive separators. The idea of decreasing pressure is incorporated if the cost of raising the pressure is assigned to the unit preceding the one requiring the higher pressure. Only the desire for 50/50 splits does not fall into the general economic heuristic. It has been programmed and tested in lieu of the cheapest-first heuristic for some problems, described later.

The assessment as to which of the candidate separators is cheapest is based on the product of two factors: (1) an estimation of the number of stages necessary (N_{ijk}) and (2) an estimation of the cost per stage (β_{ijk}),

where i and j are the specific key products for the separator k.

$$\text{Estimation of cost of unit} = \beta_{ijk} N_{ijk} \quad (2)$$

The estimated number of stages is calculated by routine STAGE.

For separators having linked countercurrent flows (e.g., distillation and extractive distillation, where the phase flows cannot be varied independently of one another) N is calculated from the Fenske-Underwood equation at total reflux (King, 1971),

$$N = \ln \left[\frac{(\text{LK})_D (\text{HK})_B}{[1 - (\text{LK})_D][1 - (\text{HK})_B]} \right] / \ln \alpha_{LK, HK} \quad (3)$$

For units with non-linked flows (e.g., extraction) N is calculated from the Kremser-Souders-Brown equation (King, 1971),

$$N = 3.03 \ln \left[\frac{.286}{1 - (F/K)} + .714 \right], \text{ assuming stripping factor} = 1.40 \quad (4)$$

Initially the values of all stage costs β are set at the arbitrarily low value of 1.00 (one dollar). This encourages testing of various types of units, and eliminates the problem of preliminary accurate estimation of the real cost. After subsequent detailed simulation of the process the estimate of the cost-per-stage weighting factor β for each unit included in the process is refined through the following equation:

$$\beta_{ijk} = \frac{\text{actual cost of unit}}{N_{ijk}} \quad (5)$$

where N_{ijk} is the original estimate from Eq. (3), and where the actual cost of the unit includes the cost of recovering the mass separating agent as a single component product by a later unit, the cost of a necessary change in the feed stream state of aggregation, and/or the cost of pumping

to a higher pressure for an immediate successor unit, if any. This "actual cost" may not be that at all if the detailed simulation reveals that the use of that particular unit caused the violation of some constraint. In that case, β_{ijk} is given a high value to discourage further use of that separator with those key products (see Chapter 5).

β_{ijk} values are often updated by groups, instead of singly, for more rapid convergence to a final process. For a given separator, k , if one β_{ijk} has been calculated by the above procedure, then all of the other β 's having the index k , regardless of keys, can be updated to a high fraction (usually 80 or 100%) of this value of β_{ijk} if those β 's have never been updated before. This helps the synthesizer to reject whole categories of unlikely candidate separators. (This group updating is not used if the β_{ijk} was set to a high value because of a constraint violation.)

The updated values of β are used in synthesizing a new process. Values of N_{ijk} are not re-evaluated once calculated, since the value is a function only of the distribution coefficients (taken as those of the feed) and of the split fraction of i and j , which do not change.

Besides the general heuristic several more specific heuristics were added to PICK as their need evolved during the course of the research. The three that were used in all examples run are described here:

- (1) If a stream contained only two mass separating agents (and no other products), PICK would often choose a separator which required another mass separating agent. Although such a choice would ultimately be corrected by subsequent evaluation, the choice in the first place is poor and warranted prevention by

requiring streams containing only mass-separating-agents to be separated by energy-separating-agent units.

- (2) Sometimes cycling would occur, wherein two separation units would alternately separate out one mass separating agent by adding the other. This is prevented by disallowing the use of the same separator with the same key products more than once in the same process.
- (3) Certain separator types are inherently more expensive than other types if the separation factors are the same in each. A study has been made comparing distillation, extractive distillation, and extraction (Souders, 1954). A heuristic based on this study is incorporated into PICK in which extractive distillation and extraction are eliminated from consideration if the separation factor between the key components is lower by 20% than the separation factor found by Souders to make the cost comparable with the cost of distillation. This only applies if distillation can effect the separation with the same key products.

Evolutionary Option

The synthesizing procedure is repeated, updating β 's until no change appears in the process structure. An option available to SYNT analyzes the units selected to determine if the presence of any separator utilizing a mass separating agent is required because a multicomponent product prohibits the use of an energy-separating-unit at that juncture. If this is the case, PROC is called (through Entry 4) to split the multicomponent

product so that an energy-separating-agent unit can be considered, as described in Chapter 3. The entire synthesis procedure is then repeated using the new product set. If this results in a process of lower total cost, the change is made permanent; else, the old product set is restored. In either case, the search for units made necessary by multicomponent products is continued through the process.

5. DETAILED SIMULATION

To evaluate the synthesized separation process and to provide feedback information for improvement in further synthesis attempts, the flow-sheet which is assembled by SYNT is simulated in detail. This simulation is directed by routine DETAIL. The primary results of the simulation are the costs--combined capital and operating--of each separator that has been chosen for the process. To provide these results, the flow rates, compositions, pressures, temperatures, and the thermal conditions of all streams must be calculated. The physical constants of all of the components are also required for sizing the units. In addition to this, various constraints on the units are checked for violation.

Essentially, DETAIL only parcels out information to various unit simulators and stores the information returned. Descriptions of these unit simulators, which include distillation, extractive distillation, liquid-liquid extraction, stripping, and absorption are in Appendix B. Each of the unit simulators requires the name (number) of the key components, key component split fractions, feed temperature, pressure, flow rate and composition. The routines also require that the components be ordered in decreasing value of their estimated distribution coefficients for that particular unit. DETAIL does its bookkeeping according to a master listing, which is arbitrarily the ordering of the components in the initial problem statement. Therefore, DETAIL must reorder all of the feed components for a particular unit simulator, including a renumbering of the key components. Of course all of the component thermodynamic properties must also be re-ordered. Successful completion of the unit simulation results in returning to DETAIL the costs of the unit and all information about the two effluent

streams. Components in the effluent streams are then reordered by DETAIL to conform to the master listing.

Most of the possible constraint violations are checked in the unit simulators themselves. DETAIL does check the effluents from single-section separation units (units where the feed enters one end of the column, wherein specifications can only be made on one key component) to ascertain if the split fractions of both key components have been met. If they have not, the separation is attempted with a two-section unit, wherein the feed enters near the middle of the column into already existing counter-current flows. This requires finding a second mass-separating-agent. For an absorber the second section is a stripper with the stripping medium supplied in the problem description. For extraction the choice is more difficult. There the counter-solvent is, somewhat arbitrarily, limited to the component present in the feed with the highest concentration as long as (1) it is not one of the key components, (2) it distributes below the heavy key, and (3) it is in a liquid state as a pure component at the prevailing temperature of the unit. If the component selected as counter-solvent is part of a multicomponent product from the process, this step will effectively result in a splitting of that product. If one or more components are present which satisfy Conditions 1 and 2 but not 3, the temperature of the unit is lowered until Condition 3 is satisfied. This, of course, requires the purchase and operation of a cooling unit, whose cost is added to the cost of the separation unit. If no suitable second mass-separating-agent can be found, it is considered a constraint violation, and simulation of that process stops. Control is returned to SYNT, which makes use of the

information gathered to that point in the simulation and prevents incorporation of the same unit with the same keys into future processes that are synthesized.

Condensers and evaporators are also added to the feed of any unit that does not have its feed in the required state of aggregation, or to any unit which requires that the feed temperature be changed from that of the available feed stream.

Simulator Constraints

A number of other conditions can prevent completion of the simulation. Some of these constraint violations are so severe as to warrant precluding the use of the unit with those specific keys in further syntheses; whereas the use of other units which violate constraints is only to be discouraged. Thus two levels of violation have been established:

- A. Constraints which permanently eliminate a separation unit with specific keys:
 - 1. Extreme flow ratios of internal counter-current streams.
 - 2. Improper phase miscibility (or immiscibility) for the type of separator.
- B. Constraints which discourage use of separator with specific keys:
 - 1. Poor estimation of ordering of component distribution coefficients for unit.
 - 2. Unit operation requires extreme temperatures.

Extreme flow ratios can occur in units with non-linked flows, such as extraction. The flow ratios are constrained to values that can be handled without

channeling or other inadequate phase contacting, or to values that do not require a column with an unreasonable aspect ratio. Volume flow ratios of ten to one, in either direction, were set as the limits.

The effluents of extractors are checked by a miscibility routine (see Appendix E) to assure that there are two immiscible liquid phases present. Likewise, the bottoms of an extractive distillation unit is required to be one homogeneous phase, and is checked by the same routine. Violation of these constraints justifies eliminating the candidate separation units with these specific keys. This is accomplished by eliminating the appropriate non-zero element in the Product Separability Matrix.

Component Ordering

Component orderings for the process flowsheet synthesis are based on the composition of the initial feed and conditions of 130°F and 14.7 psia. Because of the addition of mass separating agents to streams and the separation of other components the distribution coefficients can change so radically as to upset the component ordering that is expected in a particular unit. This behavior will then be detected since each unit simulator calculates new distribution coefficients based on the exact feed composition to the unit and the operating temperature. If these reorderings are such that components distribute on the opposite side of the keys from that expected, the isolation of the products of the chosen product set can be affected. Such a unit is clearly not wanted in that position in the process. No future use is discouraged by assigning the β weighting factor an arbitrarily high value. The only exception to this is in the case of a binary separation, where it does not matter which component distributes

above the other since they are both final products. Here DETAIL switches the ordering and the simulation proceeds. Extreme temperatures also result in the assignment of high β values. These temperature extremes are now set at 600°F and -200°F. The high value that is assigned to a β is such to make the estimated cost by Eq. (2) equal to or greater than 10^8 dollars. This also implies that any single unit which costs this amount will be recognized as a constraint violation in itself, whether or not one of the aforementioned constraints was violated.

Early Constraint Checks

Considerable computation time can be saved by identifying constraint violations as early in the synthesis procedure as possible. For constraints of Category A it is possible to check for violations in the Product Separability Matrix before SYNT begins the flowsheet synthesis. In this manner many candidate separators are eliminated before any consideration is given to them. The early check also eliminates stopping the detailed simulation in the middle of a process in many cases (see the hydrocarbon examples in Chapter 6). This identification is performed by the optional routine CHECK, which is interposed before SYNT is called the first time (see Fig. 2). Constraint A1 is also checked in STAGE. The use of early checks must be cautious because the exact composition that will exist in each unit is yet unknown. Flow ratios in any unit for any set of keys can be estimated for the distribution coefficients of the keys. Instead of 10 to 1, the flow ratio constraint is relaxed in the early checks to 20 to 1. All possible flows are considered. Miscibility checks are made for extraction and

extractive distillation by assuming a 50/50 mixture of solvent and heavy key. The temperature and distribution coefficients are those of the standard conditions.

Unit Simulators

All of the unit simulators base their sizing calculations on group methods of calculation. They incorporate many rules of thumb for sub-optimization of the unit (see Appendix D). Sizing and costing is based on equations fitting the data given by Peters and Timmerhaus (1968), as reported in Appendix D. Except where specific experimental distribution coefficients are used, all of the thermodynamic data are based on a modified regular solution theory (Weimer and Prausnitz, 1965; Halpenstill and Van Winkle, 1963), and correlations from Reid and Sherwood (1966). The program listings for these calculations are in Appendix B.

6. SAMPLE SEPARATING SCHEMES

A. Hydrocarbon SeparationsExample No. 1

Consider a feed stream containing six components, a mixture of olefins and paraffins, from which four final products are desired as indicated below. The feed rate is 100 lb moles/hour.

<u>Compound</u>	<u>Split Fraction</u>	<u>Desired Products</u>				<u>Feed Mole Fraction</u>
		<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	
Ethane	0.990	1	0	0	0	0.20
Propane	0.990	0	1	0	0	0.20
Butane	0.990	0	0	1	0	0.15
Pentane	0.990	0	0	1	0	0.15
Propene	0.990	0	0	0	1	0.15
1-Butene	0.990	0	0	0	1	0.15

Split fractions of all mass-separating-agents = 0.995

Each of the feed components as well as all potential mass-separating-agents are assigned a component number, which remains the same throughout the synthesis procedure and by which each component is identified. This numbering also forms the master listing for accounting purposes. Other input information is given in Table 6-1. This input information includes the critical pressure (PRESSURE), the critical temperature (TEMP), the normal boiling point (BOILING PT), the molecular weight (MOL WT), and a molecular structure factor (SF, where 1.0 = normal paraffin or non-hydrocarbon, 2.0 = homomorph of a normal paraffin, 3.0 = cyclic paraffin or a homomorph, 4.0 = aromatic or a homomorph). The critical compressibility factor (ZC), the molar volume (VOLUME), the acentric factor (OMEGA), parameters for the Miller-Raidel vapor pressure correlation (G, AK), and parameters for regular

TABLE 1
HEATING VALUES OF LIQUID FUELS

COMPOUND	MOLECULAR WEIGHT	HEATING VALUE, BTU PER POUND	HEATING VALUE, BTU PER GALLON	HEATING VALUE, BTU PER CUBIC FOOT	HEATING VALUE, BTU PER CUBIC INCH	HEATING VALUE, BTU PER CUBIC CENTIMETER	HEATING VALUE, BTU PER CUBIC METER	HEATING VALUE, BTU PER CUBIC FOOT	HEATING VALUE, BTU PER CUBIC INCH	HEATING VALUE, BTU PER CUBIC CENTIMETER	HEATING VALUE, BTU PER CUBIC METER
Ethane	30.07	17.89	60.1	1.30	0.00013	0.00013	1.30	1.30	0.00013	0.00013	1.30
Propane	44.10	25.09	84.3	1.87	0.00018	0.00018	1.87	1.87	0.00018	0.00018	1.87
Butane	58.12	32.29	107.4	2.34	0.00023	0.00023	2.34	2.34	0.00023	0.00023	2.34
Pentane	72.15	39.49	130.5	2.81	0.00028	0.00028	2.81	2.81	0.00028	0.00028	2.81
Hexane	86.17	46.69	153.6	3.28	0.00032	0.00032	3.28	3.28	0.00032	0.00032	3.28
1-Butene	56.10	30.89	102.9	2.21	0.00022	0.00022	2.21	2.21	0.00022	0.00022	2.21
Phenol	94.12	41.49	138.6	2.99	0.00030	0.00030	2.99	2.99	0.00030	0.00030	2.99
Methylhydrazine	44.10	25.09	84.3	1.87	0.00018	0.00018	1.87	1.87	0.00018	0.00018	1.87
Methane	16.04	13.90	46.3	1.00	0.00010	0.00010	1.00	1.00	0.00010	0.00010	1.00
Benzene	78.11	45.09	149.7	3.16	0.00031	0.00031	3.16	3.16	0.00031	0.00031	3.16
Heptane	100.20	51.89	172.8	3.63	0.00036	0.00036	3.63	3.63	0.00036	0.00036	3.63
Isopropylalcohol	60.10	33.89	112.9	2.44	0.00024	0.00024	2.44	2.44	0.00024	0.00024	2.44
Methylalcohol	32.05	18.89	62.9	1.36	0.00014	0.00014	1.36	1.36	0.00014	0.00014	1.36
Ethylalcohol	46.07	26.89	89.0	1.91	0.00019	0.00019	1.91	1.91	0.00019	0.00019	1.91
Hexamethylbenzene	120.16	58.89	196.8	4.28	0.00043	0.00043	4.28	4.28	0.00043	0.00043	4.28

COMPOUND	MOLECULAR WEIGHT	HEATING VALUE, BTU PER POUND	HEATING VALUE, BTU PER GALLON	HEATING VALUE, BTU PER CUBIC FOOT	HEATING VALUE, BTU PER CUBIC INCH	HEATING VALUE, BTU PER CUBIC CENTIMETER	HEATING VALUE, BTU PER CUBIC METER
1	30.07	17.89	60.1	1.30	0.00013	0.00013	1.30
2	44.10	25.09	84.3	1.87	0.00018	0.00018	1.87
3	58.12	32.29	107.4	2.34	0.00023	0.00023	2.34
4	72.15	39.49	130.5	2.81	0.00028	0.00028	2.81
5	86.17	46.69	153.6	3.28	0.00032	0.00032	3.28
6	100.20	51.89	172.8	3.63	0.00036	0.00036	3.63
7	114.23	57.09	191.9	4.00	0.00040	0.00040	4.00
8	128.25	62.29	211.0	4.37	0.00043	0.00043	4.37
9	142.28	67.49	230.1	4.74	0.00047	0.00047	4.74
10	156.30	72.69	249.2	5.11	0.00051	0.00051	5.11
11	170.33	77.89	268.3	5.48	0.00054	0.00054	5.48
12	184.35	83.09	287.4	5.85	0.00058	0.00058	5.85
13	198.38	88.29	306.5	6.22	0.00062	0.00062	6.22
14	212.40	93.49	325.6	6.59	0.00065	0.00065	6.59
15	226.43	98.69	344.7	6.96	0.00069	0.00069	6.96
16	240.45	103.89	363.8	7.33	0.00073	0.00073	7.33
17	254.48	109.09	382.9	7.70	0.00077	0.00077	7.70
18	268.50	114.29	402.0	8.07	0.00080	0.00080	8.07
19	282.53	119.49	421.1	8.44	0.00084	0.00084	8.44
20	296.55	124.69	440.2	8.81	0.00088	0.00088	8.81

solution theory calculations (LAMBDA, TAU, PSI) are calculated by the thermodynamic routines from the input data mentioned above.

The following separators are to be considered for this process:

<u>Number</u>	<u>Separator</u>
1	Distillation
2	Extractive distillation with phenol
3	Extractive distillation with tetrahydrofuran
4	Extractive distillation with hexene
5	Solvent extraction with benzene
6	Solvent extraction with heptane
7	Solvent extraction with isopropanol
8	Stripping with nitrogen
9	Absorption with eicosane
10	Absorption with hexamethylbenzene

Some of these agents cannot form feasible separations with the various feed components; e.g., the phases will not be immiscible in Separator No. 6. They are included to test the capability of the program to handle such situations and to offer some flexibility for the recovery of mass separating agents.

WAB is called to create a feasible product set, and finds that the desired products can be produced. This results in the following mapping of components (by the number) onto product numbers (INDEX):

Product Set No. 1:

Index = Components

1 = 3 4
 2 = 5 6
 3 = 1
 4 = 2
 5 = 7
 6 = 8
 7 = 9
 8 = 10
 9 = 11
 10 = 12
 11 = 13
 12 = 14
 13 = 15

For this product set and with the routine CHECK not being employed, SYNT synthesized fifteen processes that were rejected during detailed simulation due to constraint violations of miscibility and flow ratios. For example, extractive distillation with phenol was eliminated because phenol was found to be immiscible with the streams being processed. Extractive distillation with hexene was consistently rejected as a candidate because it did not effect a significantly better separation factor in comparison to distillation. Solvent extractions with heptane and benzene were eliminated on the basis of solvent miscibility with the feed. Finally, an acceptable process was found (Fig. 4). Furthermore, SYNT found no way of improving upon this feasible process with the given product set.

Figure 4 contains the format that will be used for presenting the rest of the processes synthesized in the examples. In the Table under the flow sheet, each separator is identified by STRM NUMB, the number of the stream which is the feed to the separator. Light key (LK) and heavy key (HK) component (COMPNT) and product (PRODUCT) numbers are identified for each separator. SEP NUM identifies the type of separator. NXT STR gives the number of the stream which is the overhead, or solvent-phase, product; the number of the second product from the unit is always one higher. MSA RCL identifies the number of the stream in which a mass separating agent used by the unit is isolated for recycle. LST STR is the number of the feed stream to the immediately preceeding unit. COST gives the unit cost in dollars, and the final columns indicate which of the products are present in the stream.

Fig. 4. Feasible process for Example No. 1 with Product Set No. 1.

STAN	CHPONT	PRODUCT	SEP	NXT	MSA	LST
NUMD	LK	HK	LK	NUM	STR	RCL
1	1	5	2	3	2	0
2	0	0	0	0	0	0
3	6	3	1	2	1	4
4	2	5	2	4	3	6
5	0	0	0	0	0	0
6	0	0	6	4	0	0
7	6	6	6	2	2	8
8	0	0	0	0	0	0
9	0	0	0	0	0	0
TOTAL 3						

COST PRODUCTS

206445	1	2	3	4
0	3			
302833	1	2	4	
1247267	2	4		
0	1			
0	4			
38829	2	6		
0	2			
0	6			

1798393

Using the routine CHECK, the number of constraint-violating processes synthesized was cut from 15 down to one, after which the same feasible process was found. The constraint violation came from a two-section extractor which was impossible to build because of extreme flow ratios. CHECK eliminated all potential No. 5 and 6 separators and many of the No. 2 and 7 separators from the Product Separability Matrix, all on the basis of improper miscibility conditions. Tighter constraints on the phase flow ratio tests in CHECK would have caused the removal of some of the absorptions. CHECK reduced the number of candidate separators making up the Product Separability Matrix from 769 to 540.

Next, focussing its attention on separators requiring mass separating agents in this acceptable process, SYNT decided to have PROD split the product containing Components 5 and 6. This multicomponent product necessitated the use of the mass separating agent. The following new product set was created:

Product Set No. 2

Index = Components

1	=	3	4
2	=	6	
3	=	5	
4	=	1	
5	=	2	
6	=	7	
7	=	8	
8	=	9	
9	=	10	
10	=	11	
11	=	12	
12	=	13	
13	=	14	
14	=	15	

The implementation of this product set by SYNT resulted in sixteen rejected processes (again because of constraint violation) followed by two feasible processes (see Figures 5 and 6), before SYNT found that it could do no better. Use of CHECK cut to two the number of constraint-violating processes synthesized before the two feasible processes. Both constraint violations came from miscibility in extraction. The final process generated from Product Set No. 2 is cheaper than the process from Product Set No. 1, even though there are more products. This is an instance of a violation of the initial heuristic that the minimum number of products is best, and will be discussed at greater length in Chapter 7.

This same example with the same specifications was rerun with two changes: (1) the 100% group updating of β for the same separator was changed to 0%, and (2) all separator types were removed except for distillation. The synthesizer created two feasible processes (and no infeasible ones) which are the same as the ones produced by the second product set above (i.e., Figs. 5 and 6). The input desired products included keeping the olefins together in a single product, but PROD found that that was not possible using the given separators (i.e., only distillation). This illustrates that PROD can function in providing product splits where required. It also shows that with a small number of separator types the synthesis procedure stabilizes very rapidly.

Example No. 2

A second mixture of hydrocarbons is discussed here as another example. This mixture consists of paraffins, olefins, and cyclic compounds.

Fig. 5. First feasible process for Example No. 1 with Product Set No. 2.

STRN	COMP	PRODUCT	SEP	NXT	HS	LST		
NUMB	LK	HK	HK	LK	NUM	STR	RCL	STR
1	5	3	1	2	1	2	0	0
2	2	6	2	5	1	4	0	1
3	0	0	0	3	0	0	0	1
4	1	5	3	4	1	6	0	2
5	0	0	0	0	0	0	0	2
6	0	0	0	3	0	0	0	4
7	5	2	5	3	1	8	0	4
8	0	0	0	0	0	0	0	7
9	0	0	0	0	0	0	0	7
TOTAL								8

COST PRODUCTS IN STREAM

341309	1	2	3	4	5
60517	2	3	4	5	
0	1	0	0		
125505	3	4	5		
0	2				
0	4				
244720	3	5			
0	3				
0	5				

772139

FIG. 6. Second and stabilized process for Example No. 1 with product Bc
No. 2.

STRM	CHPONT	PRODUCT	SEP	NXT	MSA	1ST
NUMB	LK	HK	HK	LK	NUM	STR
1	2	6	2	5	1	2
2	3	5	3	4	1	4
3	4	6	1	2	1	6
4	5	6	0	0	0	0
5	6	6	2	3	1	8
6	7	6	0	0	0	0
7	8	6	0	0	0	0
8	9	6	0	0	0	0
TOTAL \$						5

COST PRODUCTS IN STREAM

77551	1	2	3	4	5
125629	2	4	5		
246595	1	2			
0	4	2			
244762	3	5			
0	2				
0	1				
0	3				
0	5				

654537

in the range C_5 through C_7 . The compounds along with their split fractions and desired product groupings are shown in Table 6-2. The products correspond to separating the paraffins, olefins, naphthenes and aromatics from one another. The candidate separators are shown in Table 6-3. Component numbering is given below:

<u>Compound</u>	<u>Number</u>
Pentane	1
Hexane	2
Heptane	3
Benzene	4
Toluene	5
Cyclohexane	6
Hexene	7
1-Pentene	8
Phenol	9
Tetrahydrofuran	10
Hexene	11
Methyl Ethyl Ketone	12
Methyl Isobutyl Ketone	13
Isopropanol	14
Nitrogen	15
Elecene	16
Monomethylbenzene	17

Using the thermodynamic routines as in the previous example, the resulting separation orderings for each of the separators are shown in Table 6-4.

This example was run with and without group updating to 100% of the values for separators of a given type. During the course of the runs the synthesizer found it desirable to employ three different product sets, because of the use of mass-separating-agents with multicomponent products. The first product set is that corresponding to the original specification, shown in Table 6-5a. The second product set consists of splitting one multicomponent product (Table 6-5b). The third product set splits the remaining multicomponent product, leaving only single components as products (Table 6-5c).

Table 6-2. Feed ComponentsExample No. 2

<u>COMPOUND</u>	<u>SPLIT FRACTION</u>	<u>DESIRED PRODUCTS</u>						<u>FEED MOLE FRACTION</u>
		1	2	3	4	5	6	
Pentane	0.990	1	0	0	0	0	0	0.125
Hexane	0.990	0	1	0	0	0	0	0.125
Heptane	0.990	0	0	1	0	0	0	0.125
Benzene	0.990	0	0	0	1	0	0	0.125
Toluene	0.990	0	0	0	1	0	0	0.125
Cyclohexane	0.990	0	0	0	0	1	0	0.125
Hexene	0.990	0	0	0	0	0	1	0.125
3-Pentene	0.990	0	0	0	0	0	1	0.125

Split fractions of all mass-separating-agents = 0.995

Table 6-3. Candidate SeparatorsExample No. 2

<u>NUMBER</u>	<u>SEPARATOR</u>
1	Distillation
2	Extractive distillation with pheno ^l
3	Extractive distillation with tetrahydrofuran
4	Extractive distillation with hexene
5	Solvent extraction with methyl ethyl ketone
6	Solvent extraction with methyl isobutyl ketone
7	Solvent extraction with isopropanol
8	Stripping with nitrogen
9	Absorption with eicosane
10	Absorption with hexamethylbenzene

Table 6-4. Separation Ordering of Components

Example No. 2

<u>Separator No. =</u>	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>	<u>5</u>	<u>6</u>	<u>7</u>	<u>8</u>	<u>9</u>	<u>10</u>
15	15	15	15	14	14	14	14	15	15	15
8	1	1	8	9	9	9	9	8	8	8
14	2	11	14	13	13	10	14	14	11	
10	11	2	10	8	8	13	10	10	7	
11	7	7	11	10	10	8	11	11	10	
7	3	10	7	15	15	15	7	7	14	
2	10	14	12	5	5	5	2	12	2	
12	6	4	2	6	6	4	12	2	12	
4	12	12	4	7	7	6	4	4	4	
6	14	6	6	4	4	7	6	6	6	
3	4	3	3	11	11	11	3	3	3	
5	5	5	5	1	1	1	5	13	5	
13	13	13	13	2	2	2	13	5	13	
9	9	9	9	3	3	3	9	9	9	
17	17	17	17	17	17	17	16	17	17	
16	16	16	16	16	16	16	17	16	16	

Table 6-5. Product Sets for Example No. 2

a) Product Set No. 1

INDEX = COMPONENTS

1 = 4,5
2 = 7,8
3 = 1
4 = 2
5 = 3
6 = 6
7 = 9
8 = 10
9 = 11
10 = 12
11 = 13
12 = 14
13 = 15
14 = 16
15 = 17

b) Product Set No. 2

INDEX = COMPONENTS

1 = 4,5
2 = 7
3 = 8
4 = 1
5 = 2
6 = 3
7 = 6
8 = 9
9 = 10
10 = 11
11 = 12
12 = 13
13 = 14
14 = 15
15 = 16
16 = 17

c) Product Set No. 3

INDEX = COMPONENTS

1 = 5
2 = 4
3 = 7
4 = 0
5 = 1
6 = 2
7 = 3
8 = 6
9 = 9
10 = 10
11 = 11
12 = 12
13 = 13
14 = 14
15 = 15
16 = 16
17 = 17

All of the feasible processes that were synthesized for all three product sets using 100% group updating of β values are shown in Figs. 7 through 18. They are given here in the order that they were initially created. The figure numbers corresponding to the various product sets are given in Table 6-6. The underlined numbers are the figures representing the process on which the synthesizer stabilized.

Table 6-6. Processes for Product Sets with 100% Group β Updating

<u>Product Set No.</u>	<u>Figure No.</u>
1	7, 8, 9, <u>10</u>
2	11, <u>12</u> , 13, 14
3	15, 16, 17, 18

When this example was run with no group updating of β values three additional processes were synthesized for Product Set No. 1 (Table 6-5a), with the order of synthesis being Figs. 7, 19, 8, 9, 20, and 21. The synthesizer stabilized on Fig. 20. The computer attempted synthesis with Product Set No. 2 (Table 6-5b) but the synthesis did not converge, hence Product Set No. 3 was never created in this run with no group updating.

With and without the group updating of the β values the synthesizer started cycling around on all of the product sets. It would jump to and then away from a particular process. SYNT attempts to achieve stability by altering the influence of the feed flow rate to a separator on the value of β for the separator.

$$\beta = \beta / (\text{feed flow rate})^E \quad (6)$$

Normally the value of the exponent E is 0.6, but when cycling occurs SYNT increases the value of the exponent in steps of 20%. The synthesizer

STRN	CHPONT	PRODUCT	SEP	NXT	MSA	LST	COST	PRODUCTS IN STREAM
NUPB	LK	HK	HK	LN	NLP	STR	RCL	STR
1	6	3	5	E	1	2	0	0
2	7	6	6	E	2	4	6	1
3	0	0	0	0	0	0	0	1
4	7	2	4	E	1	6	0	2
5	5	5	7	E	1	6	0	2
6	1	0	2	3	3	10	18	4
7	0	0	0	0	0	0	0	4
8	6	4	1	E	2	12	17	5
9	0	0	0	0	0	0	0	5
10	0	0	0	0	0	0	0	6
11	7	10	8	E	2	14	16	6
12	0	0	0	0	0	0	0	6
13	5	9	7	E	1	16	0	6
14	0	0	0	0	0	0	0	11
15	10	9	7	E	1	18	0	11
16	0	0	0	0	0	0	0	13
17	0	0	0	0	0	0	0	13
18	0	0	0	0	0	0	0	15
19	0	0	0	0	0	0	0	15
TOTAL							2579203	

XBL 726-1192

Fig. 7. First feasible process for Example No. 2 with Product Set No. 1
--100% group updating.

STAH	CHPONT	PRODUCT	SEP	NXT	MSA	LST
NUMB	LK	HK	LK	ALM	STR	RCL
1	6	3	5	6	1	2
2	6	4	1	6	2	4
3	0	0	0	0	0	0
4	2	6	6	4	1	0
5	5	9	7	1	1	0
6	7	2	4	2	1	10
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	1	0	2	3	3	12
11	0	0	0	0	0	0
12	0	0	0	0	0	0
13	7	10	8	2	2	14
14	0	0	0	0	0	0
15	10	9	7	0	1	16
16	0	0	0	0	0	0
17	0	0	0	0	0	0

TOTAL 8

COST	PRODUCTS IN STREAM
225826	1 2 3 4 5 6
854367	1 2 3 4 6
0	5
267691	2 3 4 6
42082	1 7
718828	2 3 4
0	6
0	1
0	7
931095	2 3
0	4
0	3
82137	2 8
0	2
156361	8 7
0	8
0	7

3276387

XBL 726-1181

Fig. 8. Second feasible process for Example No. 2 with Product Set No. 1
---100% group updating.

STGH	CHPONT	PRODUCT	SEF	NKI	MSA	LST	COST	PRODUCTS IN STREAM
NUHD	LK	HK	LK	NLP	STG	RCL	STR	
1	6	3	5	6	1	2	0	225826 1 2 3 4 5 6
2	2	4	1	4	1	4	0	967989 1 2 3 4 5
3	0	0	0	0	0	0	1	0 5
4	7	2	4	2	1	0	2	709248 2 3 4
5	6	4	1	6	2	8	13	230054 1 6
6	1	8	2	3	3	10	16	931111 2 3
7	0	0	0	0	0	0	4	0 4
8	0	0	0	0	0	0	5	0 6
9	5	9	7	1	1	12	0	34569 1 7
10	0	0	0	0	0	0	6	0 3
11	7	10	8	2	2	14	17	82148 2 8
12	0	0	0	0	0	0	9	0 7
13	0	0	0	0	0	0	9	0 1
14	0	0	0	0	0	0	11	0 2
15	10	9	7	8	1	16	0	156390 8 7
16	0	0	0	0	0	0	15	0 8
17	0	0	0	0	0	0	15	0 7
TOTAL \$							3317337	

XBL 726-1191

Fig. 9. Third feasible process for Example No. 2 with Product Set No. 1
--100% group updating.

STRM	CHPONT	PRODUCT	SEP	NMT	MSA	LST	COST	PRODUCTS IN STREAM					
NUMB	LN	HK	LN	NLM	STG	RCL	STR						
1	6	3	5	6	1	2	0	225826	1	2	3	4	5
2	7	2	4	2	1	4	0	635557	1	2	3	4	6
3	0	0	0	0	0	0	0	0	5				
4	1	8	2	3	3	6	16	931396	2	3			
5	5	4	1	6	2	8	15	476664	1	4	6		
6	0	0	0	0	0	0	0	0	3				
7	7	10	8	2	2	10	17	62075	2	0			
8	2	6	6	4	1	12	0	144954	4	6			
9	5	9	7	1	1	14	0	36583	1	7			
10	0	0	0	0	0	0	0	0	2				
11	10	9	7	2	1	16	0	155929	6	7			
12	0	0	0	0	0	0	0	0	4				
13	0	0	0	0	0	0	0	0	6				
14	0	0	0	0	0	0	0	0	1				
15	0	0	0	0	0	0	0	0	7				
16	0	0	0	0	0	0	0	0	8				
17	0	0	0	0	0	0	0	0	7				
TOTAL \$							2868985						

XBL 726-1196

Fig. 10. Fourth and stabilized process for Example No. 2 with Product Set No. 1--100% group updating.

stabilized using this method on processes of Product Set Nos. 1 and 2 with 100% group updating and on Product Set No. 1 with no group updating. SYNT failed to stabilize on a process for Product Set No. 3 with 100% group updating and for Product Set No. 2 with no group updating. For 100% group updating for Product Set No. 3 the cycling was between Figures 16 and 18.

Although stability was achieved in the cases cited, the stabilized process was not the cheapest process found in all cases, even though it was by no means the most expensive. This failure of cheapest first may be related to the creation of a situation of cycling. A better method of preventing cycling is needed.

As with the example of the paraffin-olefin mixture, the product sets with a greater number of products and hence greater flexibility in choices resulted in the synthesizer finding cheaper processes in Product Set No. 2 (see Figures 11 through 14 as compared to Figures 7 through 10). Going to complete single components (Product Set No. 3) produced again higher cost processes. More on the cycling problem is discussed in Chapter 7.

B. Rare Earth Separations

Rare earth elements are separated from one another in solution. The processes that will be considered here involve the use of liquid-liquid extraction separators for the isolation of the different rare earth ions and distillation (actually evaporation) to recover the mass-separating-agent. Distribution coefficients between the aqueous phase and the organic solvent cannot be predicted well by any correlation at present (Smutz, 1970). Experimental distribution coefficients were obtained from the literature and

STN	CHPNT	PRODUCT	SEF	NXT	MSA	LST
NUMB	LK	HK	LK	NUM	STR	ACL
1	1	7	2	4	3	2
2	1	8	3	4	2	4
3	6	3	6	7	1	6
4	0	0	0	0	0	0
5	0	9	8	3	1	8
6	7	8	7	2	2	10
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	7	2	5	2	1	22
11	6	4	1	7	2	14
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	5	9	8	1	1	16
16	0	0	0	0	0	0
17	0	0	0	0	0	0

COST	PRODUCTS	IN	STREAK
89657	1	2	3
34824	3	4	
246393	1	2	5
	4		
27950	3	6	
75392	1	2	5
	6		
	3		
	8		
489104	2	5	
207917	1	7	8
	2		
	5		
	7		
37854	1	8	
	0		
	0		

TOTAL \$ 1255041

KIL 726-1193

Fig. 11. First feasible process for Example No. 2 with Product Set No. 2
 --100% group updating.

SYM	CHPONT	PRODUCT	SEP	Nx1	PSA	LSY
NUMB	LK	HK	LK	NUM	STF	RCL
1	1	7	2	4	1	2
2	6	1	4	3	1	4
3	6	3	6	7	1	6
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	7	2	5	2	1	0
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	2	6	7	5	2	10
10	0	0	0	0	0	0
11	5	6	8	1	1	12
12	6	4	1	7	2	14
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	5	5	8	1	1	16
16	0	0	0	0	0	0
17	0	0	0	0	0	0

COST PRODUCTS IN STREAM

85657	1	2	3	4	5	6	7
222670	3	4					
246353	1	2	5	6	7		
	0	3					
	0	4					
579550	1	2	5	7			
	0	6					
	0	2					
43665	1	5	7				
	0	5					
62679	1	7	0				
219208	1	7					
	0	8					
	0	7					
34782	1	8					
	0	1					
	0	6					

TOTAL \$

1590584

XBL 726-1194

Fig. 12. Second and stabilized process for Example No. 2 with Product Set No. 2--100% group updating.

STON	CHPONT	PRODUCT	SEP	NAT	MSA	LST
NUMB	LK	HK	LK	NUM	STG	RCL
1	1	7	2	4	1	2
2	8	1	4	3	1	4
3	6	3	6	7	1	6
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	6	4	1	7	2	2
7	0	0	0	0	0	0
8	2	6	7	5	1	1
9	5	9	8	1	1	1
10	7	2	5	2	1	1
11	0	0	0	0	0	0
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0

TOTAL \$

COST PRODUCTS IN STREAM

85657	1	2	3	4	5	6	7
222670	3	4					
246353	1	2	5	6	7		
0	3						
0	4						
640337	1	2	5	7			
0	6						
205959	2	5	7				
37895	1	8					
493137	2	5					
0	7						
0	1						
0	8						
0	2						
0	5						

1932007

XBL 726-1195

Fig. 13. Third feasible process for Example No. 2 with Product Set No. 2
--100% group updating.

STRN	CMPT	PRODUCT	SEP	NXT	MSA	LST	COST	PRODUCTS TN STREAM									
NUMB	LK	HK	HK	LK	ML	STP	RCL	STP									
1	1	7	2	4	1	2	0	0	85657	1	2	3	4	5	6	7	
2	8	1	4	3	1	4	0	1	222670	3	4						
3	6	3	6	7	1	2	0	1	246353	1	2	5	6	7			
4	0	0	0	0	0	0	0	2		0	3						
5	0	0	0	0	0	0	0	2		0	4						
6	6	4	1	7	2	2	13	3	640337	1	2	5	7				
7	0	0	0	0	0	0	0	3		0	6						
8	7	2	5	2	1	10	0	6	641795	2	5	7					
9	5	9	8	3	1	12	0	6	37895	1	8						
10	0	0	0	0	0	0	0	8		2	2						
11	2	6	7	5	2	14	17	8	42570	5	7						
12	0	0	0	0	0	0	0	9		0	1						
13	0	0	0	0	0	0	0	9		0	8						
14	0	0	0	0	0	0	0	11		0	5						
15	6	9	8	7	1	16	0	11	30686	7	0						
16	0	0	0	0	0	0	0	15		0	7						
17	0	0	0	0	0	0	0	15		0	8						
TOTAL \$							1947963										

XBL 726-1185

Fig. 14. Fourth feasible process for Example No. 2 with Product Set No. 2
---100% group updating.

STAN	CHPONT	PRODUCT	SEP	NXT	HEA	LST
NUMB	LK	HK	LK	NLP	STA	ACL
1	1	7	3	5	1	2
2	8	1	5	4	1	4
3	7	3	7	3	2	13
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	7	2	6	3	1	10
7	5	9	9	1	1	10
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	6	3	7	8	1	12
11	0	0	0	0	0	0
12	4	6	8	2	1	14
13	3	5	1	7	2	16
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	5	9	9	1	1	10
18	0	0	0	0	0	0
19	0	0	0	0	0	0

TOTAL \$

COST PRODUCTS IN STREAM

85657	1	2	3	4	5	6	7	0
222670	4	5						
129509	1	2	3	6	7	8		
	0	4						
	0	5						
483478	3	6						
117358	1	2	7	8	9			
	0	3						
	0	6						
274139	1	2	7	8				
	0	9						
10193785	2	8						
38665	1	7						
	0	2						
	0	8						
	0	7						
41196	1	9						
	0	1						
	0	9						

11595457

KBL 726-1183

Fig. 15. First feasible process for Example No. 2 with Product Set No. 3
--100% group updating.

STRA	CHPNT	PRODUCT	SEP	NXT	MSA	LST
NUMB	LK	HK	LK	NUM	STR	RCL
1	1	7	3	5	1	2
2	8	1	5	4	1	4
3	6	2	7	2	1	1
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	7	6	8	2	2	5
7	3	5	1	7	2	10
8	7	2	6	2	1	12
9	6	4	2	2	2	14
10	0	0	0	0	0	0
11	5	9	9	1	1	12
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	4	9	9	2	1	10
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

COST	PRODUCTS IN STREAM							
85657	1	2	3	4	5	6	7	8
222670	4	5						
246353	1	2	3	6	7	8		
0	4							
0	5							
75392	2	3	6	6				
38978	1	7						
489104	3	6						
207917	2	8	9					
0	7							
41426	1	9						
0	3							
0	6							
0	8							
35426	2	9						
0	1							
0	9							
0	2							
0	9							

TOTAL \$

1042923

XBL 726-1184

Fig. 16. Second feasible process for Example No. 2 with Product Set No. 3
---100% group updating.

STOR	CAPACIT	PRODUCT	SEP	NAT	MSA	LST
NUMB	LN	NR	LN	ALM	STR	ACL
1	1	7	3	5	1	2
2	0	1	5	4	1	4
3	6	4	2	2	2	17
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	2	6	8	6	1	2
7	4	5	1	2	1	10
8	7	2	6	3	1	12
9	6	3	7	4	1	14
10	0	0	0	0	0	0
11	5	9	9	1	1	16
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	0	0	0	0	0	0

COST	PRODUCTS IN STREAM
85657	1 2 3 4 5 6 7 8
222670	4 5
1053073	1 2 3 6 7 8
0	4
0	5
241125	3 6 7 8
91653	1 2 9
493237	3 6
93579	7 8
0	2
58012	1 9
0	3
0	6
0	8
0	7
0	1
0	9

TOTAL 8

2339006

XBL 726-1182

Fig. 17. Third feasible process for Example No. 2 with Product Set No. 3
--100% group updating.

STAN	CHPOINT	PRODUCT	SEP	MTX	MSA	LSI
NUMB	LM	HK	HK	LM	STR	RCL
1	1	7	3	5	1	2
2	0	1	5	4	1	4
3	6	4	2	8	2	6
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	6	3	7	6	1	6
7	5	9	9	1	1	10
8	7	6	8	1	1	15
9	0	0	0	0	0	0
10	4	5	1	2	1	14
11	0	0	0	0	0	0
12	7	2	6	3	1	16
13	6	9	9	2	1	18
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

COST	PRODUCTS IN STREAM
85657	1 2 3 4 5 6 7 8
222670	4 5
1053073	1 2 3 6 7 8
0	4
0	5
131243	3 6 7 8
74334	1 2 9
75405	3 6 8
0	7
57271	2 2
0	9
484269	3 6
31296	8 9
0	2
0	1
0	3
0	6
0	8
0	9

TOTAL 8

2215218

XBL 726-1168

Fig. 18. Fourth feasible process for Example No. 2 with Product Set No. 3
---100% group updating.

STAN	CHPONT	PRODUCT	SEP	NXT	MSA	LST	COST		PRODUCTS IN STREAM						
NUMB	LK	NK	LK	NK	STR	RCL	STR								
1	2	4	1	4	1	2	0	0	657374	1	2	3	4	5	6
2	7	2	4	2	1	4	0	1	709253	2	3	4			
3	6	3	5	0	1	6	0	1	275088	1	5	6			
4	1	0	2	3	3	2	16	2	931111	2	3				
5	0	0	0	0	0	0	0	2		0	4				
6	6	4	1	6	2	11	15	3	215666	1	6				
7	0	0	0	0	0	0	0	3		0	5				
8	0	0	0	0	0	0	0	4		0	3				
9	7	10	0	2	2	12	17	4	82149	2	8				
10	0	0	0	0	0	0	0	6		0	6				
11	5	9	7	1	1	14	0	6	34554	1	7				
12	0	0	0	0	0	0	0	9		0	2				
13	10	0	7	8	1	16	0	9	156390	0	7				
14	0	0	0	0	0	0	0	11		0	1				
15	0	0	0	0	0	0	0	11		0	7				
16	0	0	0	0	0	0	0	13		0	8				
17	0	0	0	0	0	0	0	13		0	7				
TOTAL									3861486						

XBL 726-1186

Fig. 19. First feasible process created using no group updating that was not created with updating--Example No. 2, Product Set No. 1.

STRM	CHPONT	PRODUCT	SEP	NXT	MSA	LST	COST	PRODUCTS IN STREAM							
NUMB	LK	HK	LK	HK	MLP	STR	RCL	STR							
1	6	3	5	6	1	2	0	0	225826	1	2	3	4	5	6
2	7	2	4	2	1	4	0	1	835557	1	2	3	4	6	
3	0	0	0	0	0	0	0	1	0	5					
4	1	8	2	3	3	6	14	2	931396	2	3				
5	2	6	6	4	2	8	13	2	45108	1	4	6			
6	0	0	0	0	0	0	0	4	0	3					
7	7	10	8	2	2	10	15	4	82075	2	8				
8	0	0	0	0	0	0	0	5	0	4					
9	5	9	7	1	5	12	0	5	62689	1	6	7			
10	0	0	0	0	0	0	0	7	0	2					
11	10	9	7	8	1	14	0	7	155929	8	7				
12	6	4	1	6	2	16	19	9	219213	1	6				
13	0	0	0	0	0	0	0	9	0	7					
14	0	0	0	0	0	0	0	11	0	8					
15	0	0	0	0	0	0	0	11	0	0					
16	0	0	0	0	0	0	0	12	0	6					
17	5	9	7	1	1	16	0	12	34789	1	7				
18	0	0	0	0	0	0	0	17	0	1					
19	0	0	0	0	0	0	0	17	0	7					
TOTAL							0		2588583						

XBL 726-1187

Fig. 20. Second feasible process created using no group updating that was not created with updating--Example No. 2, Product Set No. 1.

STRT RNUM	CH LN	POINT LN	PRODUCT LN	SEP LN	NXT LN	MSA LN	LST LN	COST	PRODUCTS	IN	STRECH
1	6	3	5	1	2	0	0	225826	1	2	3
2	6	4	1	E	2	0	1	854367	1	2	3
3	0	0	0	0	0	0	1	0	5		6
4	7	2	4	2	1	6	0	820718	2	3	4
5	5	5	7	3	1	6	0	42082	1	7	
6	1	8	2	3	10	18	4	931395	2	3	
7	2	6	6	4	2	12	17	44439	4	6	
8	0	0	0	0	0	0	5	0	7		
9	0	0	0	0	0	0	6	0	3		
10	0	0	0	0	0	0	6				
11	7	10	3	2	2	14	15	82076	2	8	
12	0	0	0	0	0	0	7	0	4		
13	6	9	7	6	1	16	0	30688	6	7	
14	0	0	0	0	0	0	11	0	2		
15	0	9	7	6	1	16	6	155932	8	7	
16	0	0	0	0	0	0	13	0	6		
17	0	0	0	0	0	0	12	0	7		
18	0	0	0	0	0	0	15	0	6		
19	0	0	0	0	0	0	15	0	7		
TOTAL \$								3147923			

KBL 726-1188

Fig. 21. Third feasible process created using no group updating that was not created with updating--Example No. 2, Product Set No. 1.

included in the input file for the synthesizer. The form of the data, not given as a function of temperature or pH, means that the extraction simulation routines cannot alter the conditions of temperature or pH if the values of the distribution coefficients of the key components obviously lead to a prohibitively expensive unit. Furthermore, since the distribution coefficients are not recalculated based on the exact composition of the feed, special steps must be taken to prohibit utilizing certain feed streams in contact with certain solvents, since the distribution coefficients will be totally erroneous. Likewise, miscible solvents are prevented from contacting in a unit.

Table 6-7 lists the feed components (Nos. 1 through 10) and the potential mass-separating-agents used in this group of examples. Since the use of different pH values in the aqueous phase leads to different distribution coefficients, the pH value was considered as part of the separator. Just as for the use of a different mass-separating-agent, a different pH can give a different ordering of the components. The first nine naturally occurring rare earths are considered, and the feed composition ratio roughly corresponds to their abundance as extracted from Monazite ore (Rare Metals Handbook, p. 398). Table 6-8 lists the separator units that are to be considered. Units 6 through 10 are back-extraction units (aqueous phase as solvent) corresponding to Units 2 through 5, respectively. All of the extraction units correspond to the "component" numberings 11 through 18 in Table 6-7, which are effectively different mass-separating-agents, although they are not all different components per se. Using the input data on the distribution coefficients (see Table 6-9), routine PROD lists the components in decreasing value of these coefficients, for each separator, as shown in Table 6-10.

Table 6-7. Component Numbering

<u>Component</u>	<u>Symbol</u>	<u>Number</u>	<u>Feed Mole Fraction</u>
<u>Feed:</u>			
Lanthanum	La	1	0.00614
Cerium	Ce	2	0.01175
Praseodymium	Pr	3	0.0015
Neodymium	Nd	4	0.00488
Samarium	Sm	5	0.00053
Europium	Eu	6	0.000025
Gadolinium	Gd	7	0.000125
Terbium	Tb	8	0.000025
Dysprosium	Dy	9	0.000025
Water		10	0.975

Mass-separating-agents:

TBP	vs. 0.266 M HNO_3	11
TBP	vs. 2.9 M HNO_3	12
TBP	vs. 12.5 M HNO_3	13
D2EHFA (.75 M in Toluene)	vs. 0.5 M HNO_3	14
0.266 M HNO_3	vs. TBP	15
2.9 M HNO_3	vs. TBP	16
12.5 M HNO_3	vs. TBP	17
0.5 M HNO_3	vs. D2EHFA	18

Changes of Molarity

As can be noted in Table 6-8, different separators operate at different pH values. Since the use of the distribution coefficients depend on the aqueous phase having the specified free acid molarity (and hence the specified pH), the feed to any unit, if it is aqueous, must have this acid molarity. If the aqueous feed is not already at this acid molarity from the previous unit, either NaOH or HNO_3 is added to the feed until the acid molarity is at the specified level. This acid or base addition results in an increase in the mole fraction of the water (and hence a decrease in the mole fraction of the rare earth ions), which is accounted for. The increase in the total salt concentration is assumed not to influence the distribution coefficients. The separator requiring the acid or base addition is

charged \$ 0.25 per pound of NaOH or \$ 0.05 per pound of HNO_3 . This cost is from the Oil Paint and Drug Reporter, and includes the cost of separation of these compounds out from the rare earths.

Table 6-8. Potential Separators

<u>Number</u>	<u>Separator</u>	<u>Feed Phase</u>	<u>Second Phase</u>
1	Distillation		
2	Solvent Extraction	0.266 M HNO_3	TBP
3	Solvent Extraction	2.9 M HNO_3	TBP
4	Solvent Extraction	12.5 M HNO_3	TBP
5	Solvent Extraction	0.5 M HNO_3	0.75 M D2EHFA in Toluene
6	Solvent Extraction	TBP	0.266 M HNO_3
7	Solvent Extraction	TBP	2.9 M HNO_3
8	Solvent Extraction	TBP	12.5 M HNO_3
9	Solvent Extraction	0.75 M D2EHFA in Toluene	0.5 M HNO_3

As alluded to previously, miscible phases are not to be contacted with one another in the extraction units. Such an occurrence is prohibited by excluding from consideration certain separators when certain products would be in the feed to those units. The forbidden product-separator combinations are listed under the examples. Because of inadequate predictability of phase miscibility, in addition to including the use of the forbidden combinations as input information, the high-level constraint routine CHECK was not used in these synthesis examples.

Initial attempts in all of the rare earth examples resulted in the solvent (water, TBP, or D2EHFA) being separated from the rare earth nitrates by distillation as a first step. The synthesizer did not know that the rare earths were required to remain in solution. This is

Table 6-9. Distribution Coefficients of Rare Earths

<u>Rare Earth</u>	<u>Into Tributyl Phosphate (TBP)</u>						<u>Into D2EHPA</u>	
	<u>0.225 M HNO₃</u>		<u>2.9 M HNO₃</u>		<u>12.5 M HNO₃</u>		<u>0.5 M HCl</u>	
	<u>D_c (1)</u>	<u>D_x</u>	<u>D_c (1)</u>	<u>D_x</u>	<u>D_c (2)</u>	<u>D_x</u>	<u>D_c (3)</u>	<u>D_x</u>
La	0.02	0.30	0.15	2.2	0.092	1.09	0.0001	0.0015
Ce	0.023	0.345	0.24	3.5	0.184	2.19	0.0025	0.0225
Pr	0.026	0.39	0.29	4.24	0.291	3.46	0.0056	0.064
Nd	0.03	0.45	0.35	5.12	0.36	4.28	0.01	0.15
Pm	0.033	0.495	0.40	5.85	0.622	7.4	0.32	0.18
Sm	0.036	0.54	0.45	6.59	1.22	14.5	0.063	0.945
Eu	0.04	0.60	0.51	7.47	2.01	25.0	0.16	2.40
Gd	0.039	0.585	0.52	7.6	2.84	33.7	0.316	4.74
Tb	0.024	0.36	0.50	7.32	6.21	73.84	1.41	21.15
Dy	0.018	0.27	0.45	6.6	8.99	106.89	3.16	47.4

$$D_c = \frac{\text{concentration in solvent}}{\text{concentration in water}}$$

$$D_x = \frac{\text{mole fraction in solvent}}{\text{mole fraction in water}}$$

(1) Peppard, et al. (1957a)

(2) Fidelis (1970)

(3) Peppard, et al. (1957b)

something unique to dissolved salts. The problem was circumvented by adding to PICK the rule that distillation (evaporation) could only be considered on streams containing two products.

Table 6-10. Component Ordering

Separator No.	1	2	3	4	5	6	7	8	9
14	11	12	13	14	15	16	17	18	19
10	12	11	11	11	10	10	10	10	10
15	13	13	12	12	16	15	15	15	15
16	14	14	14	13	17	17	16	16	16
17	6	7	9	9	18	18	18	18	18
18	7	6	8	8	9	1	1	1	1
11	5	8	7	7	1	2	2	2	2
12	4	9	6	6	2	3	3	3	3
13	3	5	5	5	8	4	4	4	4
6	8	4	4	4	3	5	5	5	5
5	2	3	3	3	4	9	6	6	6
9	1	2	2	2	5	8	7	7	7
8	9	1	1	1	7	6	8	8	8
7	18	18	18	17	6	7	9	9	9
3	17	17	16	16	14	14	14	13	13
4	16	15	15	15	13	13	13	12	12
1	10	10	10	10	12	11	11	11	11
2	15	16	17	18	11	12	3	14	14

Further synthesizing attempts then resulted in processes in which solvents extracted all of the rare earths, back-extracted all of the rare earths, and then re-extracted all of the rare earths with a new solvent. Although the learning technique of updating the β weighting factors would have eventually corrected the situation, a more direct approach was taken: Mass separating agents were forbidden to be key components in liquid-liquid extraction. This was implemented by an addition to routine PICK.

The computer routines had difficulty in predicting the latent heat for the rare earth components. This resulted in ridiculously low

costs for the evaporation separations. But since the costs of these units is so small anyhow, relative to the extractors, there is no important effect on the process synthesis.

Example No. 3 Single Rare Earth Products

As a first attempt on the rare earth separations, isolating the components as single component products was attempted. The split fractions were set at 0.95. This gave an exact equivalence between component numbers and product numbers. The forbidden separator-component combinations are shown in Table 6-11. The synthesizer failed in its assigned task of separating all of the rare earths from one another. The best that it did (Fig. 22) left one final stream containing the products 6, 7, and 13 (Eu^{+3} , Gd^{+3} , and TBP contacting 12.5 M HNO_3) for which PICK had no acceptable method of separation. The three allowable separators (Nos. 6, 7, and 8) that were not forbidden by the special product-separator list were too expensive to be used. Since SYNT found no separation method, that separation was bypassed.

Table 6-11. Forbidden Products in Separators--Example No. 3

<u>Separator</u>	<u>Product Numbers</u>							
1	0							
2	11	12	13	14				
3	11	12	13	14				
4	11	12	13	14				
5	11	12	13	14				
6	10	14	15	16	17	18		
7	10	14	15	16	17	18		
8	10	14	15	16	17	18		
9	10	11	12	13	15	16	17	18

Fig. 22. Single component rare earth separation scheme (bold lines indicate streams of the organic phase)—Example No. 3.

Four of the created processes were infeasible because they specified removing all of the rare earths from water by extraction. Although there was not a specific constraint against this, it is clearly not a desired separation. The constraint that stopped the simulation in those cases involved the split fractions of the components. A single-section unit could not meet specified split fractions of the water separation, and a second section with a counter-solvent was sought, but no suitable solvent was found. All other infeasible processes that were created were infeasible because they failed to make all of the separations, and they were extremely expensive because of the addition of acid or base.

Example No. 4 Multicomponent Rare Earth Products

In order to demonstrate the ability of the synthesizer to handle multicomponent products, several combinations of rare earths in such products were tried. In all cases where such combinations were infeasible to produce without splitting using the given separators, PROD identified them without difficulty. Two product sets that were feasible are discussed here. All of the component and separator numberings are the same as in Example No. 3. A similar set of forbidden product-separator combinations is imposed and is shown in Table 6-12. (It is not the same because the product numbering is different.)

For example No. 4 the feasible product set established by PROD is shown in Table 6-13. Among the infeasible processes that were synthesized, seven feasible processes were created, although some are very expensive because of acid or base addition. These seven processes appear in Figs. 23 through 29 in the order in which they were created. The synthesizer

STRM	CHPOINT	PRODUCT	SEP	NKT	NSA	LST	COST										PRODUCTS IN STREAM						
NUMB	LC	HK	HK	LC	NUM	STR	RCL	STR	1	2	3	4	5	6	7								
1	1	9	6	1	2	2	22	0	1028214	1	2	3	4	5	6	7							
2	4	5	4	2	8	4	14	1	28503	1	2	3	4	5	6	7							
3	10	9	4	7	1	6	0	1	264	6	7												
4	3	2	1	2	2	0	12	2	35739848	1	2	14											
5	8	5	4	5	6	10	16	2	860273	3	4	5	6										
6	0	0	0	0	0	0	0	3	0	7													
7	0	0	0	0	0	0	0	3	0	6													
8	11	3	2	8	1	12	0	4	520788	2	8												
9	17	1	1	14	1	14	0	4	198669	1	14												
10	15	8	5	12	1	15	0	5	5489	5	12												
11	5	7	3	4	6	18	20	5	39853269	3	4	8											
12	0	0	0	0	0	0	0	8	0	8													
13	0	0	0	0	0	0	0	8	0	2													
14	0	0	0	0	0	0	0	9	0	14													
15	0	0	0	0	0	0	0	9	0	1													
16	0	0	0	0	0	0	0	10	0	12													
17	0	0	0	0	0	0	0	10	0	5													
18	15	5	4	12	1	20	0	11	253483	4	12												
19	11	6	3	8	1	22	0	11	453121	3	8												
20	0	0	0	0	0	0	0	18	0	12													
21	0	0	0	0	0	0	0	18	0	4													
22	0	0	0	0	0	0	0	19	0	8													
23	0	0	0	0	0	0	0	19	0	3													
TOTAL \$									78937928														

XBL 726-1171

Fig. 23. First feasible process for Example No. 4.

STN	CHPNT	PRODUCT	SEP	NXT	MSA	LST	COST PRODUCTS IN STREAM									
NUMB	LN	HK	LN	NUM	LN	STR	ACL	STR								
1	8	9	3	5	3	2	10	0	49157	1	2	3	4	5	6	7
2	8	7	3	5	6	4	8	1	43232	3	5	9				
3	9	5	4	6	5	6	12	1	1215644	1	2	4	6	7		
4	15	8	5	12	1	8	0	2	110	5	12					
5	12	6	3	9	1	10	0	2	253	3	9					
6	14	9	6	11	1	12	0	3	7	6	11					
7	5	4	2	4	2	14	16	3	41700592	1	2	4	7			
8	0	0	0	0	0	0	0	4	0	12						
9	0	0	0	0	0	0	0	4	0	5						
10	0	0	0	0	0	0	0	5	0	9						
11	0	0	0	0	0	0	0	5	0	3						
12	0	0	0	0	0	0	0	6	0	11						
13	0	0	0	0	0	0	0	6	0	6						
14	11	5	4	8	1	16	0	7	75265	4	8					
15	3	2	1	2	3	18	20	7	3336664	1	2	7				
16	0	0	0	0	0	0	0	14	0	8						
17	0	0	0	0	0	0	0	14	0	4						
18	12	3	2	5	1	20	0	15	157116	2	9					
19	10	1	1	7	1	22	0	15	611914	1	7					
20	0	0	0	0	0	0	0	18	0	9						
21	0	0	0	0	0	0	0	18	0	2						
22	0	0	0	0	0	0	0	19	0	7						
23	0	0	0	0	0	0	0	19	0	1						
TOTAL \$							47251973									

XBL 726-1172

Fig. 24. Second feasible process for Example No. 4.

STRA	CHPONT	PRODUCT	SEP	NXT	MSA	LST
NUMD	LK	HK	LK	NUM	STR	RCL
1	3	2	1	2	3	22
2	0	3	2	5	6	14
3	10	1	1	7	1	6
4	0	9	6	5	2	8
5	6	5	4	2	6	10
6	0	0	0	0	0	0
7	0	0	0	0	0	0
8	11	0	5	8	1	12
9	15	0	6	12	1	14
10	17	3	2	14	1	16
11	5	6	3	4	7	18
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	10
17	0	0	0	0	0	10
18	16	5	4	15	1	20
19	12	6	3	9	1	22
20	0	0	0	0	0	16
21	0	0	0	0	0	18
22	0	0	0	0	0	19
23	0	0	0	0	0	19
24	0	0	0	0	0	19
TOTAL						8

COST	PRODUCTS	IN	STREAM
28092	1	2	3
1220342	2	3	4
150	1	7	5
1911062	3	6	12
35160	2	1	4
0	7	9	
0	1		
13656	5	8	
4682	6	12	
12572	2	14	
4197743	3	4	9
0	8		
0	5		
0	12		
0	6		
0	14		
0	2		
375929	4	13	
57154	3	9	
0	13		
0	4		
0	9		
0	3		
7056823			

XBL 726-1176

Fig. 25. Third feasible process for Example No. 4

STAN-CHPOINT	PRODUCT	SEP	NXT	NSA	LST
NUMB	LN	LN	LN	LN	LN
1	3	2	1	2	3
2	9	8	5	6	4
3	10	1	1	7	1
4	15	9	6	12	1
5	4	5	4	2	8
6	0	0	0	0	0
7	0	0	0	0	0
8	0	0	0	0	0
9	0	0	0	0	0
10	17	3	2	14	1
11	8	5	4	3	6
12	0	0	0	0	0
13	0	0	0	0	0
14	15	8	5	12	1
15	5	6	3	4	7
16	0	0	0	0	0
17	0	0	0	0	0
18	16	5	4	13	1
19	12	6	3	9	1
20	0	0	0	0	0
21	0	0	0	0	0
22	0	0	0	0	0
23	0	0	0	0	0

COST	PRODUCTS	IN	STREAM
28092	1	2	3
221267	2	3	4
150	1	7	
124	6	12	
17703	2	3	4
0	7		
0	1		
0	12		
0	6		
4038	2	14	
524577	3	4	5
0	14		
0	2		
2542	5	12	
6988491	3	4	9
0	12		
0	5		
371942	4	13	
121536	3	9	
0	13		
0	4		
0	9		
0	3		

TOTAL 8

ST90514

XBL 726-1173

Fig. 26. Fourth feasible process for Example No. 4.

STAN	CHPONT	PRODUCT	SEP	NXT	MSA	LST
NUND	LK	HK	LK	NUM	STR	RCL
1	3	2	1	2	3	2
2	9	8	5	6	7	4
3	10	1	1	7	1	6
4	3	9	6	2	2	8
5	8	7	3	9	6	10
6	0	0	0	0	0	0
7	0	0	0	0	0	0
8	4	5	4	2	8	12
9	16	9	6	13	1	14
10	15	8	5	12	1	16
11	12	6	3	9	1	18
12	17	3	2	14	1	20
13	11	5	4	8	1	22
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0
20	0	0	0	0	0	0
21	0	0	0	0	0	0
22	0	0	0	0	0	0
23	0	0	0	0	0	0
TOTAL 8						

COST	PRODUCTS IN STREAM						
28092	1	2	3	4	5	6	7
518366	2	3	4	5	6	9	0
150	1	7					
6158170	2	4	6	13			
427361	3	5	9				
0	7						
0	1						
655671	2	4	8				
50232	6	13					
2692	5	12					
6131	3	9					
1574671	2	14					
306744	4	8					
0	13						
0	6						
0	12						
0	5						
0	9						
0	1						
0	14						
0	2						
0	8						
0	4						
9728282							

XDL 726-1177

Fig. 27. Fifth feasible process for Example No. 4.

STAN	CHPONT	PRODUCT	SEP	NAT	NSA	LST
NUMB	LK	HK	LK	NUM	STR	RCL
1	3	2	1	2	3	2
2	4	5	4	2	8	4
3	10	1	1	7	1	6
4	17	3	2	14	1	6
5	6	5	4	5	6	10
6	0	0	0	0	0	0
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	8	9	6	5	3	12
11	5	4	3	4	7	14
12	12	8	5	9	1	14
13	15	9	6	12	1	18
14	16	5	4	13	1	20
15	12	6	3	9	1	22
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0
20	0	0	0	0	0	0
21	0	0	0	0	0	0
22	0	0	0	0	0	0
23	0	0	0	0	0	0

COST	PRODUCTS	IN	STREAM
28092	1	2	3
4976	2	3	4
150	1	7	
417	2	14	
134458	3	4	5
0	7		
0	1		
0	14		
0	2		
6518685	5	6	12
1679860	3	4	9
3209	5	9	
21110	6	12	
82886	4	13	
12813	3	9	
0	9		
0	5		
0	12		
0	6		
0	13		
0	4		
0	9		
0	3		

TOTAL \$ 8488665

XBL 726-1174

Fig. 28. Seventh feasible process for Example No. 4.

Table 6-12. Forbidden Products in Separators--Example No. 4

<u>Separator</u>	<u>Product Numbers</u>							
1	0							
2	8	9	10	11				
3	8	9	10	11				
4	8	9	10	11				
5	8	9	10	11				
6	7	11	12	13	14	15		
7	7	11	12	13	14	15		
8	7	11	12	13	14	15		
9	7	8	9	10	12	13	14	15

Table 6-13. Multicomponent Product Set--Example No. 4

<u>Index</u>	=	<u>Components</u>	
1	=	1	2
2	=	3	4
3	=	6	7
4	=	5	
5	=	8	
6	=	9	
7	=	10	
8	=	11	
9	=	12	
10	=	13	
11	=	14	
12	=	15	
13	=	16	
14	=	17	
15	=	18	

stabilized on the cheapest process that was found (Fig. 29). As a sample of the output from the detailed simulation, this entire process appears in Appendix C.

Example No. 5 Rare Earth Multicomponent Products

A second multicomponent example synthesis used the feasible product set in Table 6-14. The forbidden combinations are shown in Table 6-15.

Table 6-14. Multicomponent Product Set--Example No. 5

<u>Index</u>	<u>Components</u>
1	2 3
2	4 5
3	6 7
4	8 9
5	1
6	12
7	11
8	12
9	13
10	14
11	15
12	16
13	17
14	18

Table 6-15. Forbidden Products in Separators--Example No. 5

<u>Separator</u>	<u>Product Numbers</u>
1	0
2	7 8 9 10
3	7 8 9 10
4	7 8 9 10
5	7 8 9 10
6	6 10 11 12 13 14
7	6 10 11 12 13 14
8	6 10 11 12 13 14
9	6 7 8 9 11 12 13 14

Eight feasible processes were created; they are shown in Figs. 30 through 37, in the order in which they were first synthesized. The synthesizer stabilized on a feasible process (Fig. 36) which was considerably more expensive than the cheapest process found (Fig. 35). Here is an instance of violation of the cheapest-first heuristic. Reasons for this violation are discussed in Chapter 7.

[illegible]

COST	PRODUCTS IN STREAM					
45433	1	2	3	4	5	6
21473	3	4	10			
3189080	1	2	5	6		
	152	3	14			
	22	4	10			
1412724	1	2	9			
1657	5	6				
	0	14				
	0	3				
	0	10				
	0	4				
5089	1	11				
11652	2	9				
	0	6				
	3	5				
	0	11				
	0	1				
	0	9				
	3	2				

Fig. 30. First feasible process for Example No. 5.

XBL 726-1178

STAN	CMPT	PRODUCT	SEP	HMT	MSA	LSY
NUMB	LK	HX	HA	LK	NUM	STR
1	4	3	1	2	5	2
2	5	6	3	2	9	4
3	2	1	9	1	3	6
4	18	5	2	14	1	8
5	7	0	4	3	9	10
6	12	3	1	0	1	12
7	10	1	9	6	1	14
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	18	6	3	14	1	16
11	14	9	4	10	1	18
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

TOTAL 9

COST PRODUCTS IN STREAM

769529	1	2	3	4	5	6
409384	2	3	4	10		
1347869	1	5	6			
1317	2	14				
246168	3	4	10			
454	1	8				
1266	5	6				
0	14					
0	2					
11624	3	14				
2072	4	10				
0	8					
0	1					
0	6					
0	5					
0	14					
0	3					
0	10					
0	11					
0	4					

2789703

XEL 726-1179

Fig. 31. Second feasible process for Example No. 5.

STAN	COMPNT	PRODUCT	SEP	NXT	MSA	LST	COST	PRODUCTS IN STREAM							
NUMB	LK	HK	HK	LK	NUM	STR	RCL	STR							
1	4	3	1	2	2	2	10	0	162762	1	2	3	4	9	6
2	5	6	3	2	7	4	8	1	1007691	2	3	7			
3	0	3	1	4	5	6	12	1	533807	1	4	5	6		
4	16	5	2	12	1	8	0	2	34639	2	12				
5	11	6	3	7	1	10	0	2	5615	3	7				
6	14	9	4	10	1	12	0	3	7	4	10				
7	2	1	5	1	3	14	16	3	36884	1	5	6			
8	0	0	0	0	0	0	0	4	0	12					
9	0	0	0	0	0	0	0	4	0	2					
10	0	0	0	0	0	0	0	5	0	7					
11	0	0	0	0	0	0	0	5	0	3					
12	0	0	0	0	0	0	0	6	0	10					
13	0	0	0	0	0	0	0	6	0	4					
14	12	3	1	8	1	16	0	7	405	1	8				
15	10	1	5	6	1	18	0	7	1147	5	6				
16	0	0	0	0	0	0	0	10	6	8					
17	0	0	0	0	0	0	0	14	0	1					
18	0	0	0	0	0	0	0	15	0	6					
19	0	0	0	0	0	0	0	15	0	5					
TOTAL							8		1782757						

XBL 726-1109

Fig. 32. Third feasible process for Example No. 5.

STRN	CHPONT	PRODUCT	SEP	NXT	MSA	LST
NUMD	LN	KL	LN	STR	RCL	STR
1	4	3	1	2	4	18
2	0	4	2	4	6	4
3	2	1	5	1	3	6
4	15	9	4	11	1	8
5	5	7	3	2	6	10
6	12	3	1	8	1	12
7	10	1	5	6	1	14
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	15	5	2	11	1	16
11	15	6	3	9	1	18
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

TOTAL 8

COST PRODUCTS IN STREAM

23414	1	2	3	4	5	6
122892	2	3	4	9		
3431352	1	5	6			
135	4	11				
3816625	2	3	9			
1108	1	8				
3149	5	6				
0	11					
0	4					
5950	2	11				
10492	3	9				
0	8					
0	1					
0	6					
0	5					
0	11					
0	2					
0	9					
0	3					

7417118

XBL 726-1190

Fig. 33. Fourth feasible process for Example No. 5.

SEPARATOR 7 FOR STREAM NUMBER 11
TWO SECTION EXTRACTION
LIGHT KEY IS SM

	FEED	SOLVENT	HEAVY KEY IS EU REFLUXER	EXTRACT	RAFFINATE	LB MOLES/HR
2.9MHN03H2OVSTBP	210.67265	35530.69856	4959.67476	35526.01735	5175.22062	
	0.00000	1.00000	0.00000	.99999	.00000	
.266MHN03H2OVSTBP	.00099	0.00000	0.00000	.00001	.00000	
PR	.00000	0.00000	0.00000	.00000	.00000	
ND	.00000	0.00000	0.00000	.00000	.00000	
SM	.00001	0.00000	0.00000	.00000	.00000	
OY	.00000	0.00000	0.00000	.00000	.00000	
YB	.00000	0.00000	0.00000	.00000	.00000	
EU	.00000	0.00000	0.00000	.00000	.00000	
GO	.00000	0.00000	0.00000	.00000	.00000	
TBP2.9MHN03	.99900	0.00000	1.00000	.00000	.99901	

SURFACE TENSIONS = 5.72123E+01 6.86807E+01
 EFFICIENCY = .279 DENSITY DIFFERENCE (LB/FT³) = 120.605
 SURFACE TENSIONS = 5.72598E+01 6.86856E+01
 EFFICIENCY = .285 DENSITY DIFFERENCE (LB/FT³) = 120.578
 SECTION B PLATES = 19% DIAMETER (IN) = 120.02
 SECTION B PLATES = 200 DIAMETER (IN) = 120.06
 TOTAL CAPITAL COST = 1.67986E+06
 TEMP (F) = 100.000

SEPARATOR 1 FOR STREAM NUMBER 12
 NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.6700E+01
 PRESSURE IN DRUM = 2.96213E-13 PSIA
 FLASH DRUM WITH BOILER
 LIGHT KEY IS TBP.266MHN03 HEAVY KEY IS TB

REBOILER
 DUTY = 3.571E+06 TEMP = 100.00
 EXHAUST STEAM U=150 DELTA T = 1.200E+02 HOURLY OP COST = 8.927E-01
 REBOILER AREA = 1.984E+02 REBOILER CAP COST = 1.480E+03

	FEED	VAPOR	LIQUID	LB MOLES/HR
.266MHN03H2OVSTBP	3.57070E+03	3.57070E+03	2.21119E+04	
TBP.266MHN03	.00001	.00001	.00000	
TBP2.9MHN03	.99999	.99999	.00000	
EU	.00000	.00000	.00000	
SM	.00000	.00000	.00000	
OY	.00000	.00000	.00000	
YB	.00000	.00000	.00000	
GO	.00000	.00000	.00000	
PR	.00000	.00000	.00000	
ND	.00000	.00000	.00000	

SEPARATOR 1 FOR STREAM NUMBER 13
 NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.6700E+01
 PRESSURE IN DRUM = 1.11851E-11 PSIA
 FLASH DRUM WITH BOILER
 LIGHT KEY IS .266MHN03H2OVSTBP HEAVY KEY IS OY

REBOILER
 DUTY = 1.169E+06 TEMP = 100.00
 EXHAUST STEAM U=150 DELTA T = 1.200E+02 HOURLY OP COST = 2.923E-01
 REBOILER AREA = 6.497E+01 REBOILER CAP COST = 6.497E+02

	FEED	VAPOR	LIQUID	LB MOLES/HR
.266MHN03H2OVSTBP	1.16938E+03	1.16938E+03	7.50181E-05	
.266MHN03H2OVSTBP	.01732	.01732	.00000	
.266MHN03H2OVSTBP	.98166	.98166	.00000	
.266MHN03H2OVSTBP	.00002	.00002	.00000	
.266MHN03	.00000	.00000	.00000	
OY	.00000	.00000	.00000	
YB	.00000	.00000	.00000	
GO	.00000	.00000	.00000	
PR	.00000	.00000	.00000	
ND	.00000	.00000	.00000

STRM NUMB	COMPNT LK	HK	KK	PRODUCT LK	SEP NUM	MKT STR	MSA ACL	LST STA
1	8	7	3	4	5	2	4	0
2	14	9	4	10	1	4	0	1
3	6	5	2	3	3	4	8	1
4	0	0	0	0	0	0	0	2
5	0	0	0	0	0	0	0	2
6	12	6	3	8	1	6	0	3
7	4	3	1	2	3	10	12	3
8	0	0	0	0	0	0	0	6
9	0	0	0	0	0	0	0	6
10	12	5	2	8	1	12	0	7
11	2	1	5	1	3	14	16	7
12	0	0	0	0	0	0	0	10
13	0	0	0	0	0	0	0	10
14	12	3	1	8	1	16	0	11
15	10	1	5	6	1	18	0	11
16	0	0	0	0	0	0	0	14
17	0	0	0	0	0	0	0	14
18	0	0	0	0	0	0	0	15
19	0	0	0	0	0	0	0	15

TOTAL \$

COST PRODUCTS IN STREAM

16170	1	2	3	4	5	6
-8	4	10				
948113	1	2	3	5	6	
0	10					
0	4					
214	3	8				
366016	1	2	5	6		
0	8					
0	3					
4442	2	8				
425559	1	5	6			
0	8					
0	2					
45566	1	8				
133350	5	6				
0	8					
0	1					
0	6					
0	5					

1739447

XBL 726-1167

Fig. 35. Sixth feasible process for Example No. 5 (cheapest process synthesized using Cheapest-First Heuristic).

STRM	CHPONT	PRODUCT	SEP	MAT	NSA	LST
NUMB	LK	HK	LK	NUM	STR	RCL
1	2	1	5	1	3	2
2	3	4	2	1	8	4
3	10	1	5	6	1	6
4	17	3	1	13	1	8
5	8	4	2	4	6	10
6	0	0	0	0	0	0
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	15	9	4	11	1	12
11	5	6	3	2	7	14
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	16	5	2	12	1	16
15	12	6	3	8	1	18
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

TOTAL 3

COST PRODUCTS IN STREAM

8202	1	2	3	4	5	6
74465	1	2	3	4	8	
65	5	6				
1054	1	13				
432234	2	3	4	0		
0	6					
0	5					
0	13					
0	1					
1118	4	11				
4240427	2	3	8			
0	11					
0	4					
392258	2	12				
58087	3	8				
0	12					
0	2					
0	8					
0	3					

5197911

XBL 726-1170

Fig. 36. Seventh and stabilized process for Example No. 5.

STRM	CMPT	PRODUCT	SEP	NXT	MSA	LST
NUMB	LK	HK	LK	NUM	STR	RCL
1	2	1	5	1	3	2
2	3	4	2	1	7	4
3	10	1	5	6	1	6
4	16	3	1	12	1	8
5	8	4	2	4	6	10
6	0	0	0	0	0	0
7	0	0	0	0	0	0
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	15	9	4	11	1	12
11	5	0	3	2	7	14
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	16	5	2	12	1	16
15	12	6	3	8	1	18
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0
TOTAL						8

COST PRODUCTS IN STREAM

8202	1	2	3	4	5	6
82545	1	2	3	4	8	
65	5	6				
1432	1	12				
465640	2	3	4	8		
0	6					
0	5					
0	12					
0	1					
1264	4	11				
4580754	2	3	8			
0	11					
0	4					
434199	2	12				
65899	3	8				
0	12					
0	2					
0	8					
0	3					

5640000

XDL 726-1169

Fig. 37. Eighth feasible process for Example No. 5.

New Heuristic

To explore the logic of this example further and to search for yet a cheaper process for this example, a different heuristic was used in PICK. For each candidate separator, instead of the cheapest split, the closest split to 50/50 on the number of moles of rare earths was considered. Then the cheapest of these candidate separations was chosen. In addition to 50/50 splits, 0/100 and 100/0 were tried (i.e., one product off the top and one product off the bottom). The use of these heuristics with Example No. 4 resulted in five more feasible processes, most of them very expensive, but one-off-the-top found a process that was much cheaper than any other created (Fig. 38).

STRN	CHPONT	PRODUCT	SEP	NAT	HSP	LST
NUMB	LK	HK	LK	NLM	STR	RCL STR
1	8	7	3	4	5	2
2	14	9	4	10	2	4
3	6	5	2	2	5	6
4	0	0	0	0	0	0
5	0	0	0	0	0	0
6	16	6	3	10	1	2
7	4	3	1	2	3	16
8	0	0	0	0	0	0
9	0	0	0	0	0	0
10	12	5	2	8	1	12
11	2	1	5	1	3	14
12	0	0	0	0	0	0
13	0	0	0	0	0	0
14	12	3	1	8	1	16
15	10	1	5	6	1	18
16	0	0	0	0	0	0
17	0	0	0	0	0	0
18	0	0	0	0	0	0
19	0	0	0	0	0	0

TOTAL \$

COST PRODUCTS IN STREAM

16170	1	2	3	4	5	6
-8	4	10				
127176	1	2	3	5	6	
0	10					
0	4					
36	3	10				
88967	1	2	5	6		
0	10					
0	3					
259	2	4				
107886	1	5	6			
0	4					
0	2					
2551	1	4				
7293	5	6				
0	4					
0	1					
0	6					
0	5					

330330

XBL 726-1160

Fig. 38. Cheapest known process for Example No. 4 (created using a one-off-the-top heuristic).

7. DISCUSSION

Heuristics

The results of this dissertation work center on demonstrating the ability of a logical procedure, as programmed on the computer to synthesize separation trains. To accomplish this various heuristics of general applicability to synthesize separation trains were created and evaluated.

Incorporating heuristics into the programming was done where no algorithmic procedure could be ascertained, or where it could save considerable computation time without bypassing the goal of ability to synthesize good separation schemes. All the major heuristics have been relatively successful, but some cases where a heuristic fails to succeed have been encountered.

Fewest Feed Splits

Consider first the heuristic in PROD which favors the creation of product sets which make the least number of separations on the original feed to the process. This criterion ignores the need for subsequent separation of the mass separation agents. Therefore, the process that is finally synthesized may well have more separators than separations on the original feed. However, if in the creation of product sets separators were penalized by one full separation unit for the recovery of the mass separating agents, one would then be led to sequences which avoid mass separating agents altogether. Furthermore, as PROD is presently constructed, there is no way of distinguishing when a separation using a mass separating agent would be required.

Separators with mass separating agents are penalized in two ways in the present work. The first is through the normal change in the β weighting factor associated with that separation. Although the product set is fixed, β reflects both the cost of the separation and the cost of recovering the mass separating agent. Here the separator gets just comparison with other units--based on the actual cost of its implementation. This method of cost evaluation has in the examples run often rejected such types of separators in favor of distillation, except where a particular separation cannot be done by distillation.

The second method of mass-separating-agent penalization is a post-synthesis assessment by SYNT. Once SYNT can find no better process by updating β values, mass-separating-agent separators in the process are checked to determine if their use was required because the energy-separating-agent alternative could not generate the required product set. If this is affirmative, PROD is called to split the multicomponent product involved, so that distillation can be considered for the separation. In the hydrocarbon examples cited in Chapter 6, the implementation of this heuristic procedure resulted in a lower cost process.

As in Example No. 2, splitting a multicomponent product so that an energy-separating-agent separator can be considered does not always lead to the energy separating agent being used. (It was used in Example No. 1.) Splitting a product creates another product and allows the synthesizer to choose among a greater number of candidate key components, as well as candidate processes.

Weighting Factor β

Process improvement through the updating of weighting factors, although usually successful, has failed on occasion by cycling between two (or more) processes (e.g., Example No. 2), each using the same separators with the same key components but in different sequential ordering. The β values reflect the type of separator and the keys used but not the position of the unit in the process. The presence of non-key components in the units can radically affect the cost; consider for example, a light component necessitating refrigerated reflux. This situation has been partially corrected by normalizing the cost for updating with respect to the feed flow rate by dividing the updated cost factor β by the flow rate raised to some power, as indicated in Eq. (6). But this is really not a good solution. The estimated costs need to reflect the position of the unit in the process in some way. A good solution is yet to be found on this point.

Cheapest First

The heuristic of beginning at the feed to the process and inserting the cheapest available of the feasible candidate separators for a given group of products ("cheapest first") has been reasonably successful. The greatest advantage to a synthesis heuristic such as cheapest-first is its simplicity, both in terms of programming and in speed of computation. The justification, aside from its ease of implementation, is two-fold:

(1) The least expensive of the available separators for any given feasible key-component split is taken. This is usually a logical choice. However, under some circumstances the least expensive separator can (a)

necessitate the use of a mass separating agent whose presence in successor streams may make some or all of the units through which it passes more expensive. The separator in which it is recovered as a single component product is accounted for in the β factor, but other units are not considered.

Choosing the least expensive separation can also (b) prohibit the use of some particular separator in a downstream separation because of the physical properties of the necessary mass separation agent that was used. For example, the use of a unit may be prohibited because of improper phase (im)miscibility with a feed that contains the mass separating agent from that upstream, cheaper separator. Or, (c) one unit can discourage the use of a particular separator as a successor because of the conditions of the effluents of the predecessor (e.g., thermal condition or pH).

(d) The cheapest separator may allocate the non-key components in a way that calls for an expensive subsequent separator, while a more expensive separator would not have done this.

(2) The tightest product splits are left to be made near the end of the separation train. This is also logical if it is true that the flows into separators toward the end of the train are smaller. This is usually the case since other products will have been removed in upstream separators. The smaller flows allow for smaller internal flows in these separators, which are ones that necessitate large internal flows, relative to the feed. Such a reduction in internal flows saves operating costs on any heating or cooling of flows and capital costs on the column size.

One principal instance where cheapest-first failed to stabilize on the cheapest process that was found was in the rare earth extraction

examples (Examples Nos. 3, 4, and 5). These examples show instances of violations of all of the above-mentioned assumptions and draw-backs to cheapest-first. Rather than having the size of the streams decreasing through the separation train, the addition of solvents (and especially counter-solvents in two-section extractors) produce an increase in the flow rates of most streams. This increase also exists because the rare earths themselves represent only a small fraction of the initial feed, and the removal of several rare earths in a separator does not significantly decrease the flow rate of the remaining stream. This is a violation of Point No. 2 above. Further, the choice of a particular unit may require a great amount of solvent relative to some other unit. This material must then flow through all of the successor units of that stream, making all of the successor units more expensive (Point No. 1a). Flows also increase because of the addition of chemicals to change the pH of a feed stream to a particular unit. This pH change also runs counter to Point 1c; in fact, many of the very expensive units indicated on the figures reflect a predominant cost of acid or base addition. The flagrant violation of Point No. 1b appears in Example No. 3, where a mass separating agent is chosen which can have only one type of separator as a successor unit (Separator No. 9). This separator happened to be infeasible because of the flow ratio, and hence no separation could be made.

The other instance where the cheapest-first heuristic failed to stabilize of the cheapest process occurred in Example No. 2. In this example, without imposing some special procedure, the synthesizer would not have stabilized at all. Cycling occurred between processes, for which the only cure available is to increase the dependence of the cost of the unit

on the feed rate. In most cases this causes the synthesizer to stabilize, although not necessarily on the cheapest process. It may not be the stabilization procedure that is at fault here, but more the underlying problem of the cause of the cycling in the first place. As mentioned previously, ascribing a cost to a unit based only on the key components, the separator type, and the feed rate is apparently inadequate to predict its cost in a future process where it is in a different position relative to the non-keys.

To say that cheapest-first has failed when the synthesizer does not stabilize on a cheapest process is too sweeping. The heuristic has been able to thread its way through the myriad of possible processes to find several that are quite reasonable relative to the many processes that are prohibitively expensive, which it never needed to explore. Optimality is never expected to be guaranteed when heuristics of any type are used, anyway.

Comparison With Other Work

In comparing this procedure with that of the dynamic programming method of Hendry and Hughes (1972), a number of differences appear. Their method can be considered algorithmic whereas this work is largely heuristic. It is, however, difficult to decide where assumptions leave off and heuristics begin. The dynamic programming method must assume that any process which uses a mass separating agent will have that agent recovered in the immediate successor unit; i.e., it cannot handle mass separating agents as normal products. Since the feed composition is never known when the units are simulated (which occurs before the process is synthesized)

perfect separations must be assumed, and the distribution coefficients cannot reflect activity changes due to the presence of yet unknown components in unknown amounts. The latter is a very serious assumption if extractive distillation agents or other substances which are picked for their ability to change relative volatilities are present. In fact for the example given by Hendry and Hughes the cited reference for the data (Carmichael, 1962) shows that the amounts of the components in the mixture can actually change the separation ordering of the components. This change of relative volatilities, let alone change in ordering, cannot be handled in the dynamic programming method.

Consider next the computation time involved. Since all possible units are calculated (as binary splitters, then with three components, then with four, etc.) before the synthesis proceeds, a large number of products creates a combinatorial problem of the first magnitude. Moreover, beginning at the end of the process runs counter to the natural flow of information. It requires guessing the state-variable values that are input to the unit--temperature, pressure, and thermal condition in this case, since perfect splits on the components are already assumed. The separators must be simulated for a variety of values of these input parameters. Running the example problem given by Hendry and Hughes using the program used in this work took less than one half second on the computer, including the calculation of all necessary thermodynamic properties from the input critical properties.

With the method of the present work, beginning at the initial feed requires no assumptions about the feed conditions to the units; exact mole fractions are available. Separation factors can be calculated

based on the actual composition. All combinations of products need not be calculated as key components in all of the separators--only the ones that can lead to a feasible process are considered in the first place, and only the ones chosen are costed in detailed simulation.

As with many solutions that are guaranteed correct, the separation problem treated in the dynamic programming method is rather unrealistic, or at least limited. The method used in the present work does not guarantee an optimal solution, but it gives good answers to a real problem.

APPENDIX A

Possible Arrangements of N Separator Units Which Have One and Two Products Each

Define:

N = number of units

S_N = Number of possible connection combinations of N units

$S_0 = 1$

N units have 2N outputs of which N-1 are to be connected. Number of combinations:

$$\binom{2N}{N-1} = \frac{(2N)!}{(N-1)!(N+1)!} \quad (\text{Liu, 1968})$$

But this includes a factor of N, connecting a unit to itself

$$S_N = \frac{1}{N} \binom{2N}{N-1} = \frac{(2N)!}{N!(N+1)!}$$

Recurrence relations:

$$S_{N+1} = \sum_{i=0}^N S_i S_{N-i}$$

Limiting ratio:

$$\frac{S_{N+1}}{S_N} = \frac{2(2N+1)}{(N+2)}$$

$$\lim_{N \rightarrow \infty} \left(\frac{S_{N+1}}{S_N} \right) = 4$$

N	S_N
1	1
2	2
3	5
4	14
5	42
6	132
7	429
8	1430
9	4862
10	16796
11	58786
12	208012
13	742900
14	2674440
15	9694845
16	35357670
17	129644790
18	477638700
19	1767263190
20	6564120420
21	24466267020
22	91482563640
23	343059613650
24	1289904147324
25	4861946401452

APPENDIX B

Program Listing

RED	104
SEVERITY	105
VP	105
PROD	106
MAX	111
CHECK	112
SEPPAC	113
ACTVY	114
SOLPAR	114
MISBL	115
DGE	115
SYNT	116
PICK	119
STAGE	120
DEVAL	121
TVAP	124
ACOND	124
PUMP	124
VLA	125
DISTL	126
RMIN	128
FRAG	128
FRAGE	128
EUBL	129
LEN	129
RBI	130
REG	130
PROL	131
TOWEL	131
EXTOR	132
DEXTOR	133
ASBR	135
SXK	136
SSA	136

1	IF(LN=0) GO TO 98	IF(PJ=0) PJ=1
2	KK=K+1	END
3	P(I,J)=K	MM=1
4	PAIRS ARE REMAPPED ONTO LR = P(I,I)	KK=LR(I,PJ,M)
5	LR(LN+1)=P(LN+1)	IF(KK=0) GO TO 41
6	LR(LN+2)=P(LN+2)	NR(KK)=NR(KK+1)
7	CONTINUE	GO TO 44
8	COMBINE PRODUCT PAIRS INTO LARGEST POSSIBLE PRODUCTS	CONTINUE
9	DO 46 I=1,ND	NR(I)=NR(I)
10	ND=0	IF CHECK IF COMP ARE LISTED IN PRODUCT SET ONCE, MORE THAN ONCE, NOT
11	ND=0	AT ALL
12	DO 41 JJ=1,N	DO 42 JJ=1,N
13	IF(JJ=NR(I)) GO TO 46	IF(NR(JJ)=0) GO TO 52
14	KK=0	IF(NR(JJ)=1) GO TO 67
15	MM=1	NR(I) = NUMBER OF MULTICOMPONENT PRODUCTS IN PRODUCT SET I
16	PJ=P(I,J)	NR(I) = TOTAL NUMBER OF PRODUCTS IN PRODUCT SET I
17	IF(LR(I,PJ,M)=0) GO TO 39	NR(I)=NR(I)+1
18	KK=K+1	NR=NR(I)
19	NR=1	ADD COMP AS PRODUCTS IF NOT PREVIOUSLY LISTED
20	IF(KK=0) GO TO 41	LL=0
21	IF(KK=1) NR(I)=1	LL=LL+1
22	PJ=P(I,J)	IF(LR(I,LL+1)=0) GO TO 123
23	PK=P(I,K)	PJ=NR(I)
24	IF(LR(I,PJ,M)=0) GO TO 43	LR(I,LL+1)=JJ
25	IF(NR=0) GO TO 41	GO TO 52
26	NR=0	NR=NR(I)
27	DO 42 JJ=1,N	ELIMINATE DUPLICATION OF PRODUCTS LISTED MORE THAN ONCE
28	IF(JJ=NR(I))	DO 45 J=1,N
29	MM=MM+1	ND=0
30	IF(LR(I,PJ,M)=0) GO TO 45	J=P(I,J)
31	NR=NR+1	MM=1
32	LR(I,PJ,M)=LR(I,PK,M)	LR=LR(I,PJ,M)
33	NR=NR(I)	IF(LR=0) GO TO 85
34	DO 44 KK=NR+1	IF(LR=0) JJ GO TO 84
35	PJ=NR(I)	GO TO 48
36	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
37	NR=NR+1	LR=LR(I,PJ,M)
38	CONTINUE	LR(I,PJ,M)=0
39	IF(LR(I,PJ,M)=0) GO TO 45	IF(LR=0) GO TO 84
40	CONTINUE	CONTINUE
41	DO 46 I=1,ND	CONTINUE
42	ND=0	MM=1
43	DO 47 JJ=1,N	MM=1
44	IF(JJ=NR(I))	MM=1
45	MM=MM+1	MM=1
46	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
47	NR=NR+1	MM=1
48	CONTINUE	MM=1
49	DO 46 I=1,ND	MM=1
50	ND=0	MM=1
51	DO 47 JJ=1,N	MM=1
52	IF(JJ=NR(I))	MM=1
53	MM=MM+1	MM=1
54	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
55	NR=NR+1	MM=1
56	CONTINUE	MM=1
57	DO 46 I=1,ND	MM=1
58	ND=0	MM=1
59	DO 47 JJ=1,N	MM=1
60	IF(JJ=NR(I))	MM=1
61	MM=MM+1	MM=1
62	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
63	NR=NR+1	MM=1
64	CONTINUE	MM=1
65	DO 46 I=1,ND	MM=1
66	ND=0	MM=1
67	DO 47 JJ=1,N	MM=1
68	IF(JJ=NR(I))	MM=1
69	MM=MM+1	MM=1
70	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
71	NR=NR+1	MM=1
72	CONTINUE	MM=1
73	DO 46 I=1,ND	MM=1
74	ND=0	MM=1
75	DO 47 JJ=1,N	MM=1
76	IF(JJ=NR(I))	MM=1
77	MM=MM+1	MM=1
78	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
79	NR=NR+1	MM=1
80	CONTINUE	MM=1
81	DO 46 I=1,ND	MM=1
82	ND=0	MM=1
83	DO 47 JJ=1,N	MM=1
84	IF(JJ=NR(I))	MM=1
85	MM=MM+1	MM=1
86	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
87	NR=NR+1	MM=1
88	CONTINUE	MM=1
89	DO 46 I=1,ND	MM=1
90	ND=0	MM=1
91	DO 47 JJ=1,N	MM=1
92	IF(JJ=NR(I))	MM=1
93	MM=MM+1	MM=1
94	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
95	NR=NR+1	MM=1
96	CONTINUE	MM=1
97	DO 46 I=1,ND	MM=1
98	ND=0	MM=1
99	DO 47 JJ=1,N	MM=1
100	IF(JJ=NR(I))	MM=1
101	MM=MM+1	MM=1
102	IF(LR(I,PJ,M)=0) GO TO 45	MM=1
103	NR=NR+1	MM=1
104	CONTINUE	MM=1
105	DO 46 I=1,ND	MM=1
106	ND=0	

[illegible]

Z = 52 N = 76 A = 128

J	EJAY	EROT
0	0.	0.
1	2.05	0.02
2	1.26	0.07
3	2.05	0.13
4	1.26	0.22
5	1.87	0.33
6	1.26	0.47
7	1.87	0.62
8	2.04	0.80
9	2.41	1.00
10	2.04	1.22
11	3.13	1.47
12	3.13	1.73
13	3.13	2.02
14	3.30	2.33
15	3.30	2.67
16	3.30	3.02
17	4.33	3.40
18	4.33	3.80
19	4.45	4.22
20	4.71	4.67
21	4.71	5.13
22	5.59	5.62
23	5.59	6.13
24	5.59	6.66
25	6.74	7.22
26	6.74	7.80
27	6.74	8.40
28	7.89	9.02
29	9.90	9.66
30	10.28	10.33
31	11.05	11.02
32	11.05	11.73
33	12.20	12.46
34	13.26	13.22
35	13.26	14.00
36	14.41	14.79
37	15.86	15.62
38	16.22	16.46
39	16.22	17.33
40	17.37	18.22
41	19.39	19.13
42	19.76	20.06
43	20.54	21.01
44	20.54	21.99
45	21.69	22.99
46	22.74	24.01
47	22.74	25.06
48	23.89	26.12
49	26.30	27.21
50	26.30	28.32

```

101 100 LAG=NR
102 100 LAG=NR
103 100 LAG=NR
104 100 LAG=NR
105 100 LAG=NR
106 100 LAG=NR
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195 100 LAG=NR
196 100 LAG=NR
197 100 LAG=NR
198 100 LAG=NR
199 100 LAG=NR
200 100 LAG=NR

```

```

SUBROUTINE MAXI(J,K,N,LX)
  MAX COMP IN PRODUCT ROUTINE FOR PROD
  COMMON/PRO/RS(10,20,20),SP(20)
  COMMON/PRO/OS(10,20),SP(20)
  IS=1
  AM=0
  AN=1.E+16
  M=0
  N=0
  IF(LD.EQ.0) RETURN
  IF(OS(LD,IS).GT.AN) GO TO 4
  AN=OS(LD,IS)
  N=N+1
  IF(OS(LD,IS).LT.AM) GO TO 2
  AM=OS(LD,IS)
  LX=LX
  GO TO 3
  END

```

```

SUBROUTINE CHECK
HIGH LEVEL CONSTRAINT CHECK
COMMON/2/AC(20,20,20,17)
COMMON/3/STP(4),LAT(12),MRQ,NRR
COMMON/4/JLK(10,20,20)
COMMON/5/JO(20,17),SO(20)
COMMON/6/STP(20,20,1)
COMMON/7/D15/NK,PSR,AC(20)
COMMON/8/IFX(27),Y(27),Z(27),SUMBLA)
COMMON/9/TRANS/PPRT(20,13),Q(20)
COMMON/10/PTGR/JRD,JLK,JST,JAS,NKD,MLX,MST,MAD
D14FN=FN KK(20)
LOGICAL MISAL,ITEMP,JTEMP
INTERF=0
MMA=151
405 JLX=MLX-T
IF(MLX,EO,0) GO TO 1
CHECK INTERNAL FLOW RATIOS FOR EXTRACTION
DO 2 I=1,NK
DO 2 J=1,NRR
IF(J=1,1)
AN=1.75+QJ
MAD=
MMA=
LD=LR(1,12,J,M)
IF(LD,EO,0) GO TO 80
IF(SILO,151,GE,ANI GO TO 79
AN=OSILO,151
GO TO 78
80 IF((AN,GE,.05).AND.(AN,LT,40.1) GO TO 2
ELIMINATE THOSE WITH HIGH FLOW RATIOS
DO 1 J=1,NRR
XX(LJ)=151
2 CONTINUE
1 RT=560
IF((MLX,NKD),EO,0) GO TO 7
CHECK FOR HOMOGENEOUS LIQUID PHASE IN EXTRACTIVE DISTILLATION
DO 5 I=1,NKD
MMA=JAS-1
IF(PONT(NK,0),ST,0) GO TO 4
DO 5 J=1,NRR
PJ=PT(J)
DO 5 L=1,20
XX(LJ)=0
MAD=
01 MMA=1
LD=LR(1,12,J,M)
IF(LD,EO,0) GO TO 82
XX(LD)=XX(LD)
IF(XX(LD),LE,0.3 XX(LD)=.0001
GO TO 81
82 SJR=0
DO 3 L=1,20
SJR=SJM+XX(L)
XX(MN)=SJM+SJM
S2-I=1/(1.0+SJM)
DO 3 L=1,20
XX(L)=XX(L)+SJM
9 ITEMP=0
IF((S,LT,JLK) ITEMP=0.
JTEMP=MISAL(07,XX)
IF((ITEMP,AND,JTEMP) GO TO 4
IF((MMA,ITEMP,OR,JTEMP) GO TO 6
ELIMINATE THOSE WITH TWO LIQUID PHASES
DO 6 K=1,NRR
MK(J,K,15)=0
4 CONTINUE
7 RETURN
END

```

-113-


```
LOGICAL FUNCTION ISOLERT.XXI  
TEST WHETHER A PARTURE IS A HETEROGENEOUS PHASE.  
COMMON /XZ/ X(20),Y(20)  
DIMENSION X(20),Y(20)  
DATA TRACER,F-287
```

```
FUNCTION Z26F(K,L,RT,R)  
COMMON/414/N  
COMMON/XTANS/TC(20),TC(20),TW(20),TC(20),W(20),G(20),AK(20),EK(20)  
LG(20),DEL(20),TW(20),PC(20),V(20),D(20)  
COMMON/REG50L/A(20,20)  
DIMENSION X(20),DW(20),YV(20),C(20)
```


[illegible]

[illegible]

```

3 CONTINUE
4 IF (AM,GF,1,0F100) GO TO 99
RETURN
99 PRINT 100
MKN=99
PRINT 101,ST,MRR
110 FORMAT(F20.5)
ENCODE(55,105,APC,MRR,MRR,MRR)
PRINT APC, (K,(I,J,J=1,MRR),(JI,(M(JI,J,K),J=1,MRR),JI=1,MRR),K=
11,IST)
105 FORMAT(29H(140) SEPARATOR NO.,0,13/20X,12,9H12/12,13H(17X,12,0 *
112,4H(111)
100 FORMAT(' ERROR IN D(PK)')
101 FORMAT(21I4)
END

```

```

SUBROUTINE STAGE(LS,SN,LK,MK)
* INITIAL ESTIMATE OF NUMBER OF STAGES FOR A SEPARATION
COMMON/SEPTORZ/JAD,JL,JST,JAG,MXD,MIX,MST,MAB
COMMON/PRO/OS(20,101),SP(20)
INTEGER MK
IF (LS,GF,JLX) GO TO 6
* FENSKE-UNDERWOOD EQUATION
SN=ALOG(SP(LK)*SP(MK)/(11*-SP(LK)))+(1.-SP(MK)))/ALOG(OS(LK,15)/OS
LK,15)
RETURN
6 IF (LS,GF,JST) GO TO 7
IF (OS(MK,15),LT,10.) .AND. (OS(LK,15),GT,11) GO TO 7
SN=1000000.
RETURN
7 S=SP(LK)
T=SP(MK)
IF (LS,LI,JAG) GO TO 8
S=SP(MK)
T=SP(LK)
9 KREWSER-SOINDERS-BROWN EQUATION
SN=3. *ALOG(.286/11.-514.TIA)
FA=1.4*OS(MK,15)/OS(LK,15)
XY=11.-FA/11.-FA*LSN+1.11
IF (XY,GF,T) RETURN
SN=SN*XY
RETURN
END

```

SUBROUTINE DETAIL (I,IS,NEXT,LK,MK,NS,C,OP)

```

* STREAM NO. * COMMON /ORDN/ISOL20,101
* IS = SEPARATOR NO. * COMMON /PROP /PRPT(20,13)
* NEXT = STREAM NO. OF MORE VOLATILE EFFLUENT * COMMON /TRANS/PPRT(20,13),DI201
* NEXT+1 = STREAM NO. OF LESS VOLATILE EFFLUENT * COMMON /NAME/AN(1,20)
* LK = COMP NO. OF LIGHT KEY IN INITIAL NAMING * COMMON /SOLVT/XS(20),XA(20)
* MK = COMP NO. OF HEAVY KEY IN INITIAL NAMING * COMMON /FM/X(20),F(20),Z(20),FR,DR,RR
* NS = STREAM NO. OF RECYCLING MSA * COMMON /FLOW/F(100),FF(100),PSR(100),Q(100)
* C = CAPITAL COST OF SEPARATION(PURCHASED) * DIMENSION XX(60,20),STATE(60),STAT(2)
* OP = OPERATION COST OF SEPARATION * DIMENSION ISOH(20)
* XX = MATRIX OF COMPOSITIONS OF ALL STREAMS * COMMON /RR/AL(20),XP(20)
* MSA = MSA COMPONENT NO. * INTEGER HC
* PRPT = REORDERED MATRIX OF PHYSICAL PROPERTIES * LOGICAL MODE,MISR
* PSR = PRESSURE OF ALL STREAMS(PISA) * DATA TRACE/1,DE-10/
* P = PRESSURE(PISA) * DATA FIRST/0/
* H = ENTHALPY * DATA MS/60/
* TT = TEMPERATURE OF ALL STREAMS * DATA STAT/6MLIQUID,SHVAPOR/
* T = TEMPERATURE(DEG F) * IF(T.EQ.100) GO TO 51
* TD = TEMP OF LESS VOLATILE EFFLUENT OR BUBBLE POINT * IF(MODE) PRINT 106,IS,I
* X = COMPOSITION OF STREAM * 106 FORMAT(9, SEPARATOR *I2*,FOR STREAM NUMBER *I2)
* TD = DEW POINT * IF(TI.NE.1) GO TO 2
* Q = STATE OF AGGREGATION * FIRST PROCESS SET-UP
* 0 = VAPOR * FLAG=0
* 1 = LIQUID * IF(FIRST.EQ.1) GO TO 8
* MS = TOTAL NUMBER OF STREAMS IN PROCESS * DO 34 J=1,20
* F = FEED RATE(LB MOLES / HOUR) * 34 XX(J,J)=0
* MN = COMP NO. OF MSA * DO 1 J=1,N
* MN = TOTAL NUMBER OF COMPONENTS POTENTIALLY IN SYSTEM * 1 XX(I,J)=X(I,J)
* ISO = COMPONENT ORDERING BY DISTRIBUTION COEF * MN=MN+1ST=1
* TRACE = LOWER LIMIT OF CONCENTRATION FOR CONSIDERATION * DO 33 K=1,N
* AL = SEPARATION FACTOR * DO 33 J=1,13
* XS = COMPOSITION OF ENTERING MSA STREAM * 33 PRRT(K,J)=PRTK,K,J
* Y = COMPOSITION OF MORE VOLATILE EFFLUENT * K=MN
* Z = COMPOSITION OF LESS VOLATILE EFFLUENT * PPRT(1)
* ON = STATE OF AGGREGATION * ESTABLISH THERMAL CONDITION OF INITIAL FEED
* NLK = REORDERED COMP NO. OF LK * H=0
* NMK = REORDERED COMP NO. OF MK * T=TT(1)
* A = COMP NAME * TRPT
* ANN = REORDERED COMP NAME * H=0
* RLDATA = REAL DATA ON DISTRIBUTION COEF * CALL 91RL(X,TR,H)
* D = DISTRIBUTION COEF FOR EXTRACTION * IF(TR.GE.T) GO TO 14
* PR = PHYSICAL PROPERTIES OF COMPONENTS * TD=T
* FR = FEED RATE (LB MOLES / HOUR) * CALL DEMIX(TD,H)
* KS = REORDERED COMP NO. OF MSA * IF(TD.LF.T) GO TO 28
* AD = FLOW RATE OF MSA STREAM FOR EXTRACTIVE DISTILLATION * Q(1)=0
* SP = SPLIT FRACTION * GO TO 8
* TCH = TEMP OF TOTAL CONDENSER * 14 Q(1)=0
* FAC = SPLIT FRACTION ACHIEVED * GO TO 8
* XA = COMPOSITION OF COUNTER SOLVENT STREAM * 28 Q(1)=1
* NST = COMP NO. OF COUNTER SOLVENT OR STRIPPING AGENT * FIRST STREAM SET-UP
* KNST = REORDERED KST * 8 FIRST=1
* COMMON /LAST/ISS(100,8) * NO 13 KK=24MS
* COMMON /RLDATA/RLDATA(20,10) * F(KK)=0
* COMMON /SEPTOR/JXD,JLX,JST,JAR,MXD,MLX,MST,MAB * Q(KK)=0
* COMMON /PRO/OS(20,10),SP(20) * PSR(KK)=0
* COMMON /EXEC/400P * TT(KK)=0
* COMMON /DTSK/KP,ACT(20) * 13 CONTINUE
* COMMON /SIMP/N,IST,IPP,MRR,MRR * *
* FINAL PROCESS REPTON
* IF(OP.EQ.-10.) GO TO 2
* DO 20 KK=2,MS

```

```

DO 29 J=1,20
29 XX(KK,J)=0.
NN=IS+NN-1
Y=YY(I)
IF(IS.FO.I) NN=0
IF(C.NE.-10.1) GO TO 67
SPECIAL REVERSE ORDERING OF KEYS FOR BINARY DISTILLATION
DO 61 J=1,NNN
ISOM(J)=ISO(J,1)
X(J)=XX(I,J)
IF(X(J).LT.TRACF) X(J)=0.
DO 61 I=1,13
PRRT(J,I)=PRT(J,I)
61 K=NNN
FLAG=1.
TAT=130.
IF(T.GT.130.) TAT=T
CALL PRAC(TAT,LE,HK,9.9,9,DE,DU)
IF(AL(K).GT.AL(HK)) GO TO 65
J=HK
HK=LK
LK=J
65 DO 69 M=1,NNN
XM=0.
DO 64 K=1,NNN
IF(AL(K).LE.XM) GO TO 64
XM=AL(K)
64 MXX=K
CONTINUE
AL(MXX)=0.
69 ISO(M,1)=MXX
8 SYRQW SET=UP
67 DO 17 J=1,20
XS(J)=0.
X(J)=0.
V(J)=0.
17 Z(J)=0.
C=0.
CC=0.
OP=0.
LG=0
PR=F(I)
QN=Q(I)
N5T=0
REORDERING OF COMPONENTS FOR UNIT SIMULATOR
23 K=0
DO 4 J=1,NNN
JJ=ISOM(I,1)
IF(XK(I,JJ).GT.TRACE) GO TO 76
IF(JJ.FO.NN) GO TO 76
IF(JJ.FO.NST) GO TO 76
IF(JJ.FO.LK) GO TO 76
IF(JJ.FO.HK) GO TO 76
GO TO 4
K=K+1
X(K)=X(I,JJ)
XS(K)=X(NS,JJ)
IF(JJ.FO.NN) KS=K
IF(JJ.FO.NST) KNST=K
IF(JJ.FO.LK) NLK=K
IF(JJ.FO.HK) NHK=K
DO 37 I=1,9
ANM(I,K)=A(I,I,JJ)
O(K)=RDATA(JJ,IS)
9 DO 10 I=1,15
PRRT(K,I)=PRT(JJ,I)
10 CONTINUE
4 IF(NST.NE.0) GO TO 21
P=PSR(I)
SUM=0.
DO 5 J=1,K
SIM=SUM+X(J)
DO 6 J=1,K
X(J)=X(J)/SUM
6 SIMULATOR SELECTION
7 IF(IS.FO.1) GO TO 11
IF(IS.LT.JLX) GO TO 12
IF(IS.LT.JST) GO TO 15
IF(IS.LT.JAR) GO TO 18
GO TO 20
* EXTRACTIVE DISTILLATION
12 IF(X(KS).GE..66) GO TO 24
IF(ON.NE.0.) ON=.9
IF(XS(KS).LT..9) XS(KS)=1.
* ADD MSA UP TO X = .666
AD=FR(I)-X(KS)*2.
DO 9 J=1,K
X(J)=X(J)+FR+XS(J)*AD
FR=FR+AD
IF(MODE) PRINT 100,AD,(ANM(I,KS),I=1,9)
SUM=0.
DO 27 J=1,K
SIM=SUM+X(J)
DO 28 J=1,K
X(J)=X(J)/SUM
27 CONTINUE
26 X(J)=X(J)/SUM
24 CONTINUE
11 CALL VLG(NLK,NHK,Y,TB,SP(LK),SP(HK),QN,600.,C,OP)
Q(NEXT)=QN
GO TO 40
* EXTRACTION
19 IF(QH.NE.0.) CALL TCONDIX,FR,T,CC,OP)
TCN=0
IF(XS(KS).EQ.0.) XS(KS)=Y.
IF(MODE) LG=1
MODE=.4F
CONTINUE
CALL EXTOR(NLK,T,SP(LK),T,5,C)
TB=T
IF(LG.EQ.2) GO TO 16
C=0.
FAC=RRWZ(NHK)/(FR+X(NHK))
IF(LG.FO.1) MODS=.T.
LG=2
IF(FAC.GP.SPI(HK)) GO TO 35
0 DUAL SECTION EXTRACTION
0 SEARCH FOR COUNTER SOLVENT
T=YN
TIT=T
TX=1.000.

```

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5 USE FEED COMP OF HIGHEST MOLE FRACTION WHERE TEMP IS BELOW
9 ITS BUBBLE POINT - IF NONE, LOWER TEMP
48 AM=0.
K=500
CHK=CHK+1
IF (K,LT,CHK) GO TO 66
DO 91 J=CHK,K
IF (J,EQ,KS) GO TO 31
IF (AM,GT,X(J)) GO TO 31
TR=7
M=0.
DO 42 J=1,K
XA(J)=0.
42 XA(J)=1.
CALL QHLL(XA,TX,H)
IF (TX,LT,T) GO TO 31
AM=X(J)
TX=TX-10.
KS=J
31 CONTINUE
IF (KS,NE,0) GO TO 49
TX=5.
GO TO 48
49 DO 32 J=1,K
52 XA(J)=0
XA(KS)=1.
IF (TX,LT,T) CALL TCOND(XA,FR,TXX,CC,OP)
CALL DEXTORINLK,NHK,T,SP(LK),SP(HK),1,5,C)
TR=T
16 Q(NEXT)=0.
GO TO 40
* STRIPPING
18 IF (ON,NE,0.) CALL TCOND(XA,FR,T,CC,OP)
IF (XS(KS),EQ,0.) XS(KS)=1.
CALL DEXTORINLK,T,SP(LK),SP(HK),1,5,C)
TR=T
FAC=PROZ(NHK)/(PROZ(NHK))
IF (FAC,GT,SP(HK)) GO TO 19
IF (MODE) PRINT 107,SP(HK),FAC
107 FORMAT('...STRIPPER CANT MEET HE SPLIT FRACTION OF',F6.3,'. IT GETS
1 ONLY',F6.3)
GO TO 59
Q(NEXT)=1.
GO TO 40
* ABSORPTION
20 IF (XS(KS),EQ,0.) XS(KS)=1.
IF (MODE) LG=1
COND=0.
IF (ON,NE,1.) CALL TVAP(XA,FR,T,CC,OP)
CALL ABSORINLK,T,SP(LK),SP(HK)
TR=T
IF (LG,EQ,2) GO TO 23
FAC=PROZ(NHK)/(PROZ(NHK))
IF (LG,EQ,1) MODE=1.
LG=2
IF (FAC,GT,SP(HK)) GO TO 46
* ABSORBER-STRIPPER
Q(NEXT)
IF (NST,EQ,N7) GO TO 41

```

```

* REORDER COMPONENTS
NST=7
GO TO 25
21 DO 22 J=1,K
XA(J)=XS(J)
22 XS(J)=0.
IF (XA(KS),EQ,0.) XA(KS)=1.
XS(KST)=1.
TOT(T)
IF (ON,NE,0.) CALL TCOND(XA,FR,T,CC,OP)
CALL DEXTORINLK,NHK,T,SP(LK),SP(HK),2,5,C)
TR=T
23 Q(NEXT)=1.
40 CONTINUE
IF (C,GE,100000000.) GO TO 54
C=C*CC
IF (IS,LT,1) GO TO 46
IF (IS,GT,1) GO TO 46
* CHECK MISCIBILITY OF EXTRACTIVE DISTILLATION BOTTOMS
RT=TR+ABO.
IF (MISL(RT,2)) GO TO 46
IF (MODE) PRINT 104
C=1,F=10
GO TO 54
* BOOKKEEPING OF EFFLUENT STREAM PROPERTIES
46 Q(NEXT+1)=0.
F(NEXT)=DR
F(NEXT+1)=BR
TT(NEXT)=T
TT(NEXT+1)=TR
PSR(NEXT)=P
PSR(NEXT+1)=P
L=0
* DISTRIBUTION OF COMPONENTS IN EFFLUENT STREAMS
DO 50 J=1,NMN
JJ=ISO(J,T)
IF (X(J,J),GE,TRACE) GO TO 60
IF (JJ,EQ,44) GO TO 60
IF (JJ,EQ,NST) GO TO 60
IF (JJ,EQ,LK) GO TO 60
IF (JJ,EQ,HK) GO TO 60
XX(NEXT,JJ)=0.
XX(NEXT+1,JJ)=0.
GO TO 50
L=L+1
50 XX(NEXT,JJ)=Y(L)
XX(NEXT+1,JJ)=Z(L)
CONTINUE
IF (FLOG,NE,1.) GO TO 54
DO 68 J=1,NMN
ISO(J,1)=ISO(J)
68 DO 55 J=1,20
X(J)=0.
55 Z(J)=0.
RETURN
41 IF (MODE) PRINT 99
54 C=100000000.
GO TO 54
56 IF (MODE) PRINT 155

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      GO TO 59
50 PRINTING
      CONTINUE
      N=J+1
      LG=N(J)+1
      STAYE(J)=STAYE(LG)
      DO 52 J=1,N5,10
      IF (E(J),LE,0.) GO TO 55
      K=J+9
      PRINT 101,(M,N5,J,K),(F(M,N5,J,K),(Y(M,N5,J,K),(PSR(M,N5,J,K),(STA
      ITE(M,N5,J,K)
      DO 52 L=1,N5N
      DO 56 M=J,K
      IF (XX(M,L).NE,0.) GO TO 57
56 CONTINUE
      GO TO 52
57 PRINT 103,(A(I,L),I=1,2),(XX(M,L),N=J,K)
58 CONTINUE
59 PRINT 102
      RETURN
      SUBROUTINE TVAP(X,FR,T,CC,OP)
      COST EVAPORATOR
      DIMENSION X(20)
      H=0.
      CALL DEVIX(T,H)
      T=10.
      ORR=FR*H
      CALL RQL(T,OR,CC,OP)
      RETURN
      END

      GO TO 52
57 PRINT 103,(A(I,L),I=1,2),(XX(M,L),N=J,K)
58 CONTINUE
59 PRINT 102
      RETURN
      SUBROUTINE TCOND(X,FR,T,CC,OP)
      COST TATAL CONDENSER
      DIMENSION X(20)
      H=0.
      CALL RHL(X,T,H)
      T=10.
      QC=FR*H
      CALL REGI(T,QC,CC,OP)
      RETURN
      END

100 FORMAT(* ERROR IN DETAIL IN ATTEMPTING ABSORBER STRIPPER*)
101 FORMAT(* FOR THE FOLLOWING DISTILLATION*9.3* LB MOLES/HR OF *,
102 19A7,* HAS BEEN ADDED AS AN EXTRACTIVE SOLVENT*)
103 FORMAT(11A) STREAM NUMBER,17,9111/* FEED RATE *10611,3/* TEMPER
104 1ATURE,(F*10F11,3/* PRESSURE(PSIA)*10F11,3/* STATE*12X,10A11)
105 FORMAT(1H1)
106 FORMAT(* *2A7,-1P,10F11,4)
107 FORMAT(* ...BOTTOMS EFFLUENT NOT MISCIBLE PHASE*)
108 FORMAT(10I10)
109 FORMAT(* CANNOT FIND A REFLUXING SOLVENT - GIVING UP PROCFS*)
110 END
      FUNCTION PUMP(T,P1,P2,F)
      COST INTER UNIT COMPRESSOR
      HP=1,ORF=0.5*F*1/ALOG(P2/P1)
      CAP=549.9*HP**,.744
      OR=0.0294*HP
      PUMP=CAP+OP
      RETURN
      END

```

```

SUBROUTINE VLQ(LK,HK,T,TR,DLK,BHK,QQ,TSPEC,C,OP)
COMMON/FM/X(20),Y(20),Z(20),FR,DR,RR
COMMON/EXEC/MODE
COMMON/DIS/N,P,ACC(20)
COMMON/NAME/NAME(13,20)
1 INTFGR HK
2 ALLI=VRANK(I)+ACCHKI/(VPI(I)+ACC(I))
3 CALL FOR DISTILLATION TOWER
4 CALL DISTILL(LK,HK,T,TR,DLK,BHK,QQ,TSPEC,C,OP)
5 IF LESS THAN ONE STAGE USE FLASH
6 IF(CNF=10) RETURN
7 VV=DLK*BHK/(1-LK)*V(1-BHK)
8 VV=1/VV
9 VLV=1/ALOG(VV)
10 FAC=BHK/Z(1-BHK)
11 TP=V*1
12 DO 10 J=1,10
13 SUM=0
14 RT=1+660
15 CALL ACTVITY(T,Z)
16 DO 21 I=1,N
17 AAP=AC*(I)
18 Z(I)*X(I)=AA/(AA+1)
19 SUM=SUM+Z(I)
20 DO 22 I=1,N
21 Z(I)=Z(I)/SUM
22 CALL ACTIVITY(T,Z)
23 ALGP=1/ALOG(A(LK))
24 T=TP
25 RT=1+660
26 CALL ACTVITY(T,Z)
27 ALGP=1/ALOG(A(LK))
28 T=TPP
29 FUNC=(ALG-YLV)/(T-TP)/(ALG-ALGP)
30 IF(FUNC*GF*40) FUNC=40
31 IF(FUNC*LT=35) FUNC=35
32 T=T-FUNC
33 IF(ABS(FUNC),LT,.01) GO TO 25
34 T=TPP
35 ALGP=ALG
36 CONTINUE
37 PRINT 108,T,P
38 FORMAT(* NONCONVERGENCE IN VLQ TEMP **F10.3* PRESSURE **F10.4)
39 DO
40 QR=PRESSUM
41 QR=QR-QR
42 DO 26 I=1,N
43 VLI=LK(T+SER=Z(1)PRR)/PR
44 PR=Z(1)*ACCH(I)+VP(I,T)
45 PRINT 106,P
46 FORMAT(* PRESSURE IN DRUM **F12.5* PSIA*)
47 IF(P*LT=5) GO TO 2
48 IF(P*GT=10) GO TO 17
49 IF PRESSURE TOO LOW USE DISTILLATION ANYWAY
50 T=130
51 CALL DISTILL(LK,HK,T,TR,DLK,BHK,QQ,TSPEC,C,OP)
52 RETURN
53 H=0
54 CC=1000

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IF(QQ,FR=1) GO TO 18
CALL DEF(V,T,H)
CONTINUE
5 ROILER
6 OR=4808
7 IF(MODE) PRINT 100
8 IF(MODE) PRINT 119,(ANML(I,LK),I=1,3),(ANML(I,HK),I=1,3)
9 FORMAT(* FLASH DRUM WITH ROILER*)
10 CALL RBLIT=OP,C,OP)
11 GO TO 20
12 PARTIAL CONDENSER
13 CALL RHL(Z,T,H)
14 QCH=RR
15 IF(MODE) PRINT 101
16 IF(MODE) PRINT 119,(ANML(I,LK),I=1,3),(ANML(I,HK),I=1,3)
17 FORMAT(* PARTIAL CONDENSER*)
18 IF(I,T,85) GO TO 19
19 OP=OP+0.1E-06*QC
20 AC=QC/2500
21 CON=28*AC*.75
22 CC=CON
23 IF(MODE) PRINT 102*QC*AC*CON*OP
24 GO TO 20
25 CALL RFGIT=OP,C,OP)
26 IF(MODE) PRINT 103*FR,DR,RR,(ANML(I,I),I=1,3),X(I),Y(I),Z(I),I=1
27 1,N)
28 T=RT
29 RETURN
30 T=100
31 P=10.7
32 H=1000
33 GO TO 5
34 FORMAT(* DUTY **E10.3* AREA **E10.3* DFLTA T=16.8 TFMP
35 1**E6.2** CAP COST **E10.3* HOURLY OP COST **E10.3)
36 FORMAT(*X**FEED VAPOR LIQUID*/26X*YE12.5** LB MOLES/
37 HR*/S 23AT*YE12.5)
38 FORMAT(LK)*LIGHT LFY IS *3AT* HEAVY KEY IS *3AT)
39 CONTINUE
40 END

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SUBROUTINE DISTLLK, HK1, T9, DLK, RHK, QD, TSPEC, C, OP,
0  DISTILLATION SIMULATION
COMMON/EXEC/MODE /DIS/NOACC(20)
COMMON/FM/X(20),Y(20),T(20),FR,DR,RR
COMMON/RH/AL(20),XRL(20)
COMMON/TRANS/PC(20),TC(20),TN(20),T(20),X(20),G(20),AK(20),FK(20)
1,OHMI(20)
COMMON/ANM/ANM(1,20)
INTERSECT
LOGICAL MODE
REAL NM
# 1K = LIGHT KEY COMPONENT NO.
# HK = HEAVY KEY COMPONENT NO.
# T = TEMPERATURE OF FEED (DEG F)
# T9 = TEMP. OF DISTILLATE (DEG F)
# T9 = TEMPERATURE OF BOTTOMS (DEG F)
# DLK = SPLIT FRACTION ON LIGHT KEY
# RHK = SPLIT FRACTION OF HEAVY KEY TO BOTTOMS
# QD = THERMAT CONDITION OF FEED
# QD = THERMAT CONDITION OF DISTILLATE
# TSPEC = MAX TEMP IN REBOILER
# C = CAPITAL COSTS
# QD = OPERATING COST
# N = NUMBER OF COMPONENTS
# P = PRESSURE (PSIA)
# X = MOLE FRACTIONS OF FEED
# Y = MOLE FRACTIONS OF DISTILLATE
# Z = MOLE FRACTIONS OF BOTTOMS
# FR = FEED RATE (LB. MOLES/HOUR)
# DR = DISTILLATE RATE (LB. MOLES / HOUR)
# BR = BOTTOMS FLOW RATE (LB. MOLES / HOUR)
# AL = RELATIVE VOLATILITY OF C-1
# NM = MIN NUMBER OF PLATES
# RM = MIN REFLUX RATIO
# H9 = LATENT HEAT IN BOTTOMS
# H1 = LATENT HEAT IN DISTILLATE
# QC = CONDENSER DUTY (BTU / HOUR)
# PCT = FRACTION OF CRITICAL PRESSURE OF MIXTURE
# QD = OPERATING COST OF CONDENSER
# TC = TEMP DIFFERENCE, LOG MEAN
# AC = AREA OF CONDENSER (SQ. FT)
# CON = CAPITAL COST OF CONDENSER
# OR = HEAT DUTY OF REBOILER (BTU / HOUR)
# OR = OPERATING COST OF REBOILER
# SN = ACTUAL NUMBER OF IDEAL STAGES
# VIS = VISCOSITY OF LIQUID IN COLUMN (CP)
# EFF = OVER ALL PLATE EFFICIENCY
# NS = ACTUAL NUMBER OF PLATES
0  Q=0
0  TSPEC=2000
0  PCT=0
0  KPR=0
0  P=14.7
1  CALC RELATIVE VOLATILITIES
12 CALL PRTCAL, C, HK1, DLK, RM, NM, QD
0  CHECK FOR RAD COND DISTRIBUTION
0  QD=1E-14
0  IF (AL(1)/AL(2)) GO TO 13
13 CONTINUE
0  DO 19, I=HK1, N
0  IF (AL(I), I=1) GO TO 19
0  CONTINUE
0  IF (C, QD, T9) 50 TO 2
0  IF (NM, GEAR, L, QD, T9) 2
0  C=10
0  RETURN
0  CONTINUE
0  CALC DISTRIBUTIONS OF NON KEY COMPONENTS
0  CALL PRTCAL(NLV, NM)
0  CALC MINIMUM REFLUX:
0  CALL RM, NM, AK, QD, RM
0  IF (RM, EQ, 0.1) GO TO 32
0  CALC INTERVAL FLOWS
0  VAL=380224344.1
0  FOR PRESSURE COLUMN
0  IF (KPR, EQ, 0.1) CALL PRCL(QD, PCT)
0  REBOILER TEMP AND HEAT LOAD
0  H9=1
0  CALL QH9L(Z, T, H9)
0  TR=1
0  DISTILLATE TEMP
0  IF (QD, EQ, 1) GO TO 7
0  H9=0
0  CALL H9L(Y, T, H9)
0  QC=H9RV
0  TR=1
0  IF (KPR, EQ, 0.1) GO TO 7
0  CHECK FOR HIGH TEMP
0 23 IF (T9, GT, TSPEC) GO TO 6
0  IF (T9, GT, 120) GO TO 7
0  PRESSURE COLUMN
0  KPR=1
0  T=130
0  GO TO 12
0  P=0
0  VACUUM COLUMN
0  TR=1, QD=TSPEC
0  RT=TR+QD
0  CALL ACTVITY(RT, Z)
0  DR=1E+10
0  P=RT(1)/QD(1, T9, ACC(1))
0 4 PLATE PRESSURE DROP
0  P=0.074511NM
0  CHECK FOR MINIMUM PRESSURE
0  IF (P, LT, 1E-5) GO TO 1
0  IF (TR, EQ, 1) 2
0  RECALC RELATIVE VOLATILITIES AT NEW TEMP
0  GO TO 12
0 7 IF (MODE) PRINT 100, (ANM(I), LK), I=1, 3), (ANM(I), HK1), I=1, 3), FR, DR,
0 100, (ANM(I), T), I=1, 3), X(1), Y(1), Z(1), I=1, N)
0  IF (MODE) PRINT 102, QD
0  C=0
0 5 Z E AND COST CONDENSER
0  IF (QD, NE, 0) GO TO 8
0  VAPOR DISTILLATE = PARTIAL CONDENSER
0  H9=1
0  T=1
0  CALL DENYV, T9, H9

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      GC=HNS(V=NR)
      IF(P=NF,OPT) GO TO 4
      CALL RFL(TD,OC,C,OC)
5    GO TO 10
      IT=95/(LOG((TD-89.1)/(TD-115.1))
      OC=0.17F-06*OC
      AC=OC/(175.*TT)
      IF(AC<LT,0.) AC=0.
      CON=25.*AC*80.75
      IF(MORE) PRINT 103,GC,AC,IT,TD,CON,OC
      C=C+CON
      C=C+CON
      OR=NRV
      IF(OR<LT,0.) OR=0.
      CALL RFL(TB,OC,C,OR)
0    GILLILAND CORRELATION FOR NUMBER OF PLATES
      BE=1.563*(LOG((1.13+9.12/BE)))*0.13-1.223
      SN=(N+BE)/(1.-BE)
      OC=CELL CORRELATION OF PLATE EFFICIENCY
      SA=0.
      SB=0.
      DO 3 I=1,N
      EAC=SORTIN(111)*TC(111)*3.13*PC(111)*0.667
      SA=SA+Y(I)*FAC
      SB=SB+2111REAC
      VIS=0.00079*(SA/(TD+60.))*3.9 + 59/(TB+60.))*3.9)
      EFF=0.363/VIS*0.66
      IF(EFF<GT,1.) EFF=1.
      IF(MORE) PRINT 112,SN,EFF
      NS=SN/EFF+.99
      SIZE AND COST UNIT
      CALL TOWER(TS=V,C,DR=OC,NS,OP)
      CO=0
      T=TD
      RETURN
100  FORMAT(' DISTILLATION? 1=X,2=LIGHT KEY IS *3A7* HEAVY KEY IS *
      19A7/33XFEED DISTILLATE 33XTONS*/27X3E12.5* LB HOLES/HRS/
      2I* *3A7*3E12.5)
102  ERMALIS MINIMUM SEELIY RATIO *E12.5)
103  FORMAT(' CONDENSER *3A 7UTY *3E10.3* AREA *3E10.3* DEL
      17A1 *3E10.3* TEMP *3E6.2 * CAP COST *3E10.3* HOURLY
      2JP COST *3E10.3)
117  FORMAT(' EQUILIBRIUM STAGES *3E10.2* EFFICIENCY *3E10.5)
1    CONTINUE
      PRINT 99
99   FORMAT(' HIGH TEMP ELIMINATES DISTILLATION)
      C=C+10
      RETURN
15   PRINT 98
90   FORMAT(' SEPARATION ORDERING FOUND NOT TO BE AS EXPECTED)
      IF(MORE) PRINT 111,(AL(111)=1,N)
111  FORMAT(20.7)
32   C=10000000.
      OP=0.
      RETURN
31   C=C+10
      OP=0.
      RETURN
      END

```

```

1  CALC DIMENSION OFFLUX FROM UNDERWOOD EQUATION
2  COMMON /XZ/AL(20),XZ(20)
3  COMMON /YV/XY(20),Y(20),Z(20),FR+NR,RR
4  COMMON /D13/AA
5  DIMENSION XA(20)
6  INTEGER IK
7  DO 1 I=1,N
8  XA(I)=X(1)-AL(1)
9  NT=0
10  KR=KK
11  PHI=AL(IK)
12  NO=KX-1
13  NR=NR+1
14  DO 2 I=1,N
15  US=0
16  SUM=0
17  IF(ND,LT,1) GO TO 2
18  DO 4 I=1,NO
19  AP=AL(I)-PHI
20  S=XA(I)/AP
21  SP=SA+S/AP
22  US=US
23  IF(ND,GT,N) GO TO 5
24  DO 5 I=NO,N
25  AP=AL(I)-PHI
26  S=XA(I)/AP
27  SS=SP+S/AP
28  US=US+S
29  S=XA(I)/SS
30  PHI=(PHI+AP*(Y(S)+XA(I)*Y(1))/(Y(1)+1)
31  IF(ABS(PHI-PHI(1),LT,.000020)) GO TO 6
32  PHI=PHI
33  CONTINUE
34  PHI=PHI
35  IF((PHI,LT,AL(1K)) .AND. (PHI,GT,AL(5N))) GO TO 12
36  NT=NT+1
37  IF(NT,GT,1) GO TO 11
38  IF(NT,GT,2) GO TO 13
39  IF(XI,GT,3) GO TO 10
40  GO TO 10
41  SUM=0
42  DO 7 I=1,N
43  SUM=SUM+XA(I)*Y(I)/AL(I)-PHI
44  RV=SUM+1
45  IF(RV,LT,.0385) RV=.0385
46  RETURN
47  KR=KK
48  GO TO 1
49  PHI=AL(IK)+S*AL(HK)/2
50  KR=LK
51  GO TO 19
52  PHI=(AL(LK)+AL(HK))/2
53  KR=HK
54  GO TO 19
55  CONTINUE
56  PRINT 99
57  RETURN
58  FORMAT(10,ERRROR RUM,N)
59  END

```

```

SUBROUTINE BUSL(X,Y,XII,H)
      DIMENSION P(10),TRANS(20),TC(20),TN(20),ZC(20),W(20),G(20),AK(20),KF(20)
      COMMON /T/S/M,AAC(20)
      I=GA(20),J=L(20),TV(20),P(10),V(20),N(20)
      COMMON /D/S/A,CAC(20)
      D1=FMSIY X(20),GX(20),PA(20),PO(20)
      D2=FMSIDY YX(20)
      DO 1 I=1,N
        Y(I)=XY(I)
        IF(K(I).LT=.99991) X(I)=0.
      CONTINUE
      T=TT+460.
      FTR=14.7
      CALL ACTIVITY(T,X)
      DO 3 J=1,10
        XJP=0.
        SKDP=0.
        ISIT,L,F,ZD,I,T=20.
        DO 2 I=1,N
          TR=T/TC(I)
          IF(TR.GT.2.) GO TO 9
          TR=T*TR
          PR(I)=EXP(-G(I)/TR*(1.-TR+AK(I)*(%+TR*(1.-TR)*%))
          GX(I)=G(I)/(1.+TRR+SK(I)(1.-TRR)*PR(I)
          GO TO 14
        PR(I)=EXP(15.18*TR*(1.-TR)-1.)
        GX(I)=1.18*TR*(1.-TR)*AC(IG(I))-1.)
      CONTINUE
      XP(I)=Y(I)*P/(PR(I)*CAC(I)+AC(I)*%*(T/T))
      SKP=SKP+XP(I)
      SKD=SKD+XP(I)*GX(I)/T
      XX=ALOG(SKD)+SKP/SKD
      TP=T/I.-XX
      IF(ABS(T-TP).LT=.01) GO TO 4
      T=TP
      PRINT 99
      FORMAT(' EPOCH DEMO')
      I=TP
      DO 10 I=1,4
        ISIT=GX(I)*XD(I),GT,.991 GO TO 11
      CONTINUE
      GO TO 12
      NAC=NAC+1
      IF(NAC.GT.30) GO TO 30
      DO 7 I=1,N
        CX(I)=XP(I)
      GO TO 1
      SH=0.
      IF(M.FD.0.) GO TO 6
      DO 5 I=1,N
        S=-SH+CX(I)*TC(I)*SX(I)*%*T(ABS(T.-PR(I)/(T/TC(I))*%))
      GO TO 8
      DO 2 I=1,N
        SH=SH+TA(I)*TC(I)*SX(I)*%*T(ABS(T.-PR(I)/(T/TC(I))*%))
      SH=SH/DI
      H=SH*1.9872
      ITT=I-460.
      RETURN
      END

```

	SUBROUTINE REBLLT(QR,CC,QR)		SUBROUTINE REB(I,QR,CC,QR)
	SIZE AND COST REBOILER		COST REFRIGERATION UNIT AND ASSOCIATED HEAT EXCHANGER
	COMMON/EXEC/MODE		COMMON/EXEC/MODE
	LOGICAL MODE		LOGICAL MODE
	CR=.		DT=10.
	IF(QR.LT.0.1 OR Q=.		IF(I.T.65.) GO TO 2
	IF(MODE) PRINT 105,QR,T		IF(I.T.44.) GO TO 3
105	FORMAT(8, 'REBOILER' / ' DUTY =*,E10.3,* TEMP =*,F7.2)		IF(I.T.3.) GO TO 4
	IF(I.T.25.) GO TO 3		CR=.,25-0.6*CR
	IF(I.T.37.) GO TO 4	2	GO TO 5
	IF(I.T.45.) GO TO 5		CR=1.35-0.6*CR
C	DOWHTRM		CR=2.7*CR-0.6*
	CR=0.934*CR+0.33		GO TO 6
	CR=0.65-0.6*CR	3	CR=2.085-0.6*CR
	IF(I.T.18.)		GO TO 5
	IF(MODE) PRINT 100,CR		CR=1.64F-0.6*CR
100	FORMAT(8, 'DOWHTRM U=60 DELTA T = 30 CAP COST =*,E10.3,* HOUR	4	CR=0.6*2.7-0.6*10.55-0.00625*11
	LY OP COST =*,E10.3)	6	CR=0.6/1500.
	GO TO 6		CR=28.*CR+0.75
3	CR=0.235-0.6*CR		IF(MODE) PRINT 100,T,CR,CC,CR,CR
	DT=22.*T	100	FORMAT(8, 'REFRIGERATION UNIT', ' TEMP =*,F8.2,* CAP COST =*
	UT=150.*T		1.*E10.3 /' COND DUTY =*,E10.3,* AREA =*,E10.3,* DELTA T = 10
	IF(MODE) PRINT 101,DT,CR		2U = 150. COND CAP COST =*,E10.3,* HOURLY OP COST =*,E10.3)
101	FORMAT(8, 'EXHAUST STEAM U=150 DELTA T =*,E10.3,* HOURLY OP COST		CC=CC+CR
	1 =*,E10.3)		RETURN
	GO TO 6		END
A	CR=0.55-0.6*CR		
	DT=338.*T		
	UT=100.*T		
	IF(MODE) PRINT 102,DT,CR		
102	FORMAT(8, '100PSIA STEAM U=100 DELTA T =*,E10.3,* HOURLY OP COST		
	1 =*,E10.3)		
	GO TO 6		
5	CR=0.65-0.6*CR		
	DT=62.*T		
	UT=60.*T		
	IF(MODE) PRINT 103,DT,CR		
103	FORMAT(8, '500PSIA STEAM U=60 DELTA T =*,E10.3,* HOURLY OP COST =		
	1 =*,E10.3)		
6	IF(I.T.50000.) UT=50000.		
	AR=CR/UT		
	CR=28.*AR+0.75		
	CC=CC+CR		
	IF(MODE) PRINT 104,AR,CR		
104	FORMAT(8, 'REBOILER AREA =*,E10.3,* REBOILER CAP COST =*,E10.3)		
	RETURN		
	END		

```

SUBROUTINE PRC(IG,PCT)
  COST PRESSURE COLUMN
  COMMON/ENX(X(20),Y(20),Z(20),ER,DR,RR
  COMMON/TRANS/PC(20),TC(20),TN(20),ZC(20),W(20),G(20),AK(20),KF(20)
  1,GA(20)
  COMMON/DIS/N,P,AC(20)
  DIMENSION S(20),XZ(20)
  DD=0
  DP=0
  PP=0
  TA(20)
  RT=500
  CALL ACTIVITY(IG,T)
  DO 1 J=1,N
    1 DB=X(11)*V(11)*AC(11)
    IF(PP.LT.115) GO TO 3
    VAPOR DISTILLATE
    DO 5 I=1,N
      XZ(I)=V(11)
    5 XZ(I)=V(11)
    DO 7 J=1,15
      CALL ACTIVITY(IG,XZ)
      SUM=0
      DO 2 I=1,N
        2 SUM=SUM+S(I)
      P=1/SUM
      IF(ABS(DP-PP).LT.0.1) GO TO 8
      DP=PP
      DO 6 I=1,N
        6 XZ(I)=S(I)*P
      7 CONTINUE
      8 LIQUID DISTILLATE
      9 Q(1)
      IF(PP.LT.14.7) P=14.7
      PCT=0
      MAX PRESSURE
      DO 4 I=1,N
        PCT=PCT+V(I)*PCT(I)
        PCT=0.6*PCT
      IF(PP.GT.PCT) P=PCT
      RETURN
  END

```

```

SUBROUTINE TOWER(I,V,C,DR,DC,NS,OP)
  COST DISTILLATION TOWER
  COMMON/EXEC/MODE,ZDIS,N,B
  COMMON/FIX/X(20),Y(20),Z(20),PR,DR,RR
  COMMON/TRANS/PC(20),TC(20),TN(20),ZC(20),W(20),G(20),AK(20),KF(20)
  1,GA(20)
  LOGICAL MODE
  DL=65
  2 WAD
  DO 2 I=1,N
    WA=20+Z(11)*W(11)
    DG=WD*V(110.75)/(T+60.1)
    VX=0.1725*SQRT(DL/DG-10)
    DIAMETER
    G(1)=0.7335*SQRT(VX*TA+60.17/(2*VX*11)
    NS=NS
    IF(NS.GT.50) NS=20*NS-50
    COST=FL*AT*(NS)*.2*DIA**1.2*(1+.475*(1.-P/14.7))**2
    TEMPFAC=1
    IF(T.GE.-20) GO TO 39
    LOW TEMP COST
    TEMPFAC=1.43
    IF(T.GE.-20) GO TO 39
    TEMPFAC=2.12
    IF(T.GE.-150) GO TO 39
    TEMPFAC=3.7
    COST=TEMPFAC*100
    C=C+COST
    DP=DC+DR
    IF(MODE) PRINT 110,NS,DIA,P,COST,C,OP
    OPY=25.*350.*OP
    IF(MODE) PRINT 100,OPY
    100 FORMALIN YEARLY OPERATING COST IS **,E9.2)
    110 FORMAT(15,' PLATES DIAMETER **E10.3,'IN PRESSURE **E10.3,'PSIA
    1 TOWER COST **E10.3,' TOTAL CAPITAL **E10.3,' TOTAL OPERATING
    2 **E10.3,')
    RETURN
  END

```



```

PH=SCAMV(HK)=XAH/(1+FAH-1.1
13 CONTINUE
EXHL=EXBIANAFAL
EXH=EXHP(ANAFAM)
XLA1=EL(1)=FHH
XHA1=FHH(1)=FHH
XLA1P=FLAFALXENH
XHA1P=CHAFALXENH
OPEX=XLA1XHA1=PAHXHA1(XHA1)/(XLA1PDXHAT=XLA1XHA1P)
RAACXLA1/XHA1
137 FORMAT(6G20.5)
IF(AN=LT.0.) AN=0.
40 IF(OIP=GT.AN). GO TO A7
AN=AN-DIF
NT=NT+1
IF(NT=GT.30) GO TO 30
IF(ABS(RAAXHA1-XLA1)GE.001XLA1) GO TO 13
NT=0
IF(XLA1=LT.0.) GO TO 41
IF(XLA1=GT.0.) GO TO 40
14 NT=0
22 (XHB=XSH+(Z(HK)=XSH)*(1.-FHH*(RN+1.))/(1.-FHA)
XLB=XSL+(Z(LK)=XSL)*(1.-FHL*(RN+1.))/(1.-FHL)
NT=NT+1
IF(NT=GT.30) GO TO 30
21 XHA1=(XHB(FB=FR*(HK))/(FA
XLA1=(XLB(FB=FR*(LK))/(FA
RAA=XLA1/XHA1
IF(XLA1=GT.1.) GO TO 42
XHA1P=PHCHAFHAFEXHP(RN+1.)(AFHHA)
XLA1P=PHCLAFHAFEXHP(RN+1.)(AFHLA)
DIF=XHA1(XLA1-RAAXHA1)/(XLA1PDXHAT=XLA1XHA1P)
RN=RN-DIF
IF(RN=LT.0.) RN=0.
NT=NT+1
IF(NT=GT.30) GO TO 30
IF(ABS(RAAXHA1-XLA1)GE.001XLA1) GO TO 14
15 IF(ABS(XHA1-XHA1P)LT.01XHA1) GO TO 16
RA=BAR(SORT(XHA1/XHA1P)
NT=NT+1
IF(NT=GT.30) GO TO 30
GO TO 13
A7 OIF = DIF/2
GO TO 48
16 AN=
RN=
FAS=FA/5
SPB=5/FA
DISTRIBUTION OF COMP
SMB=0.
DO A=1,N
FAS=FA/F(I)
SPB=SPB/(I)
FLOG=(A+1)*ALOG(FAS)
IF(FLOG=GT.600.) FLOG=600.
FLG=(A+1)*ALOG(SPB)
IF(FLG=GT.600.) FLG=600.
H=(1.-FXD(FLOG))/(1.-FAC)
R=(CRO-EXP(FLG))/(1.-SPB)

```

```

Y(I)=X(I)*F(I)/(H=1.1X5(I)+(FR*(I)+FAOX(I)+SPX(I)-FQX(I))/
10(I)=RO(S)/(H=RO)
SUM=XHMY(I)
VSH=V*5
FB=FA+FAAS-V
DO 5 I=1,N
V(I)=Y(I)/SUMY
2(I)=(CXS(I)-V*Y(I)+FA*Y(I)+FR*X(I))/FR
IF(LK=GT.2) GO TO 5
IF(LAG) GO TO 32
DO 82 J=1,20
X(J)=0.
82 X(J)=0.
CHECK FOR IMMISTALE PHAGES
SKIN=
SR=0.
DO 26 I=1,N
X(I)=Y(I)*V+FA*X(I)
XBI=X(I)*FR+SRXS(I)
SXT=X+X(I)
SXB=SR+XBI
DO 28 I=1,N
X(I)=X(I)/SXT
28 XBI=XBI/SXB
IF(MISS(LRT=XI).OR.MISS(LRT=XBI)) GO TO 25
92 CONTINUE
FORMAT PRINT 101,IANM(I),LK(I)=1,3,IANM(I),NK(I)=1,3,FR,5,
1FA,V,FR,(IANM(I),I=1,3),X(I),X5(I),X(I),Y(I),Z(I),I=1,N)
COST COLUMN
CALL SXH(FA,F,V,XA,V,DMA,NSA,COSTA)
CALL SXH(FB,F,S,Z,XS,DWB,NSB,COSTB)
GO TO 10
40 RA=SRAB(I,XLA1)
NOT=NOT+1
IF(NT=GT.30) GO TO 30
GO TO 14
41 RA=SPRA
NOT=NOT+1
IF(NT=GT.30) GO TO 30
GO TO 14
42 RN=RN*2
GO TO 22
23 AN=AN/2
GO TO 13
5 CALL SSALA(FA,T,V,XA,Y,L,K=EL(K),DMA,NSA,COSTA)
IF(COSTA=GT.100000000.) GO TO 50
CALL SSALA(FB,T,S,Z,XS,L,K=DL(K),DWB,NSB,COSTB)
IF(COSTB=GT.100000000.) GO TO 50
IF(MODE) PRINT 103,IANM(I),LK(I)=1,3,IANM(I),NK(I)=1,3,FR,5,FA
1,V,FR,(IANM(I),I=1,3),X(I),X5(I),X(I),Y(I),Z(I),I=1,N)
COST=COSTA+COSTB
40 NSTNSA=NSB
IF(NT=GT.30) COST=COST+COST-50=7.2DMA*1.2*(1+ABS(I)-P/14.7)
10.2
TEMP=ACCL
LOW TEMP COST
IF(TAGE=20.) GO TO 39
TEMP=ACCL*49
IF(TGE=70.) GO TO 39
TEMP=ACCL*2.12

```

```

IF(T,GF,=150.) GO TO 10
TEMP=3.7
30 COST=TEMP*AC*YOST
IF(MODE) PRINT 102,NS,DM,NS,COST
IF(MODE) PRINT 100,T
RETURN
25 PRINT 105
30 CONTINUE
3 COST=1.E+10
GO TO 54
93 COST=100000000
94 IF(MODE) PRINT 106,T,TA,TD,EL(K),E(HK),D(LK),D(HK),SFA,FA,V
RETURN
101 FORMAT(//NO SECTION EXTRACTION//10X*LIGHT KEY IS *3A7* HEAVY KEY
1 15 *3A7/2X*FEED SOLVENT REELINER EXTRACT RAEFINATE
2 14MOLES/HR/25X,5F12.5/(1 *3A7,5F12.5/1)
102 FORMAT(//SECTION A PLATES ==15,* DIAMETER(IN) ==F10.2/* SECTI
3N 9 PLATES ==15,* DIAMETER(IN) ==F10.2/* TOTAL CAPITAL COST ==
2*E20.5)
103 FORMAT(//ABSORBER STRIPPER//10X*LIGHT KEY IS *3A7* HEAVY KEY 15*
13A7/2X*FEED SOLVENT REELINER EXTRACT RAEFINATE
2 14MOLES/HR/25X,5F12.5/(1 *3A7,5F12.5/1)
104 FORMAT(//TEMPERATURE==F10.1)
105 FORMAT(//MISCIBLE CONTACTING PHASES*)
106 FORMAT(//TEMP==G10.4* DP==G10.4* F(LK)=G10.4* E(HK)=G
11),G/* D(LK)=G10.4* D(HK)=G10.4* SFA=G10.4* FA=G10.4* V=G10.4)
21
END

SURROUNTING ABSORBER, T, D, L, S, COST;
SIMULATION OF ABSORPTION
COMMON/EXEC/MODE /15/NA,3,AC/201
COMMON/FM/X(20),Y(20),Z(20),FR,OR,PR
COMMON/SOLVT/XS(20),XAL(20)
COMMON/TRANS/OPRT(20,1),D(20)
COMMON/NAH/ANM(13,20)
H=0
TB=T
CALL SUBL(XS,TA,H)
H=0
TBT
CALL DEWL(X,TD,H)
RT=460
IF(T,GE,TB) OR (T,LE,TD) GO TO 3
CALL ACTVY(T,XS)
DO 5 I=1,N
D(I)=A*(1)*VO(I,T)
S=1.4*FR*D(LK)
KREMSER EQUATION
ANALOG(.3/1-DLK*(X(I)/Y(LK)-XS(LK)*D(LK)))+.71/.356
SC=5/FR
DISTRIBUTION OF COMPONENTS
SUMV=0
SUMZ=0
DO 2 I=1,V
Y(I)=XS(I)+D(I)+X(I)-XS(I)*D(I)+(-SE/D(I))/(1-SE/D(I))*IAN+
11.1)
SUMV=SUMV+Y(I)
Z(I)=XS(I)+X(I)-Y(I)/SF
SUMZ=SUMZ+Z(I)
2
DR=FR*SUMV
BR=35/MZ
DO 5 I=1,N
X(I)=Y(I)/SUMV
Z(I)=Z(I)/SUMZ
5
CALL SSA(AN,BR,TA,DR,Z,Y,LK,D(LK),DM,NS,COST)
IF(COST,GE,100000000.) GO TO 7
IF(MODE) PRINT 101,ANM(I,LK),I=1,3,FR,S,DR,OR,IANM(I,T,I)=1
1,3,X(I),XS(I),Z(I),Y(I),I=1,N)
* EXCESSIVE PLATE COST
IF(NS,GF,50) COST=COST+COST-7.2*50.*DM*.1,2
IF(MODE) PRINT 102,NS,DM,COST
IF(MODE) PRINT 103,T
RETURN
3
COST=1.E+10
IF(MODE) PRINT 106,T,TA,TD,BR,OR
106
FORMAT(//TEMP=G10.4* TA=G10.4* DR=G10.4* LTQ=G10.4* VAP=G10.4
1)
RETURN
101
FORMAT(//ABSORBER//10X*LIGHT KEY IS *3A7/2X*FEED GAS SOLVENT
1 IN SOLVENT OUT GAS OUT 14MOLES/HR/25X,4F12.5/(1 *3A7,
24F12.5/1)
102
FORMAT(//PLATES ==15,* DIAMETER(IN) ==F10.2/* CAPITAL COST ==
1*E20.5)
103
FORMAT(//TEMP(F) ==F10.1)
END

```


APPENDIX C

Sample Output

From Example No. 2 138

From Example No. 4 144

STN	COMP	PRODUCT	SEP	MTY	RSP	LSY	PRODUCTS IN STREAM															
NUMB	LN	WK	LN	LN	NUM	STM	RCL	STM	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	6	3	9	6	1	2	0	0	1	2	2	2	2	2	2	2	2	2	2	2	2	2
2	7	2	4	2	1	4	0	1	1	2	2	2	2	2	2	2	2	2	2	2	2	2
3	8	0	0	0	0	0	0	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2
4	1	0	0	0	0	0	0	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2
5	2	6	4	4	2	3	13	2	1	4	5	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	4	3	0	0	0	0	0	0	0	0	0	0	0	0	0
7	7	10	0	2	2	10	15	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0
9	5	7	1	1	12	0	0	5	1	6	7	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
11	10	9	7	0	1	14	0	0	0	7	0	0	0	0	0	0	0	0	0	0	0	0
12	6	4	1	6	2	16	11	5	1	6	6	6	6	6	6	6	6	6	6	6	6	6
13	0	0	0	0	0	0	0	9	7	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	12	7	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	12	6	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	9	7	1	1	10	0	12	1	7	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	17	7	0	0	0	0	0	0	0	0	0	0	0	0	0

SEPARATOR 1 FOR STREAM NUMBER 1

DISTILLATION

LIGHT KEY IS CYCLOHEXANE

HEAVY KEY IS HEPTANE

FEED DISTILLATE BOTTOMS
1.0000E+07 7.0000E+02 0.0000E+00 LB MOLES/HR

1-PENTENE .02500 .16667 .00000
PENTANE .12500 .16667 .00000
HEXENE .12500 .16667 .00000
HEXANE .12500 .16667 .00000
CENESE .12500 .16667 .00000
CYCLOHEXANE .12500 .16667 .00000
HEPTANE .12500 .00167 .00000
TOLUENE .12500 .00000 .00000

MINIMUM REFLUX RATIO = 6.34553E-02

CONDENSER

QDUT = 1.978E+07 AREA = 6.089E+03 DELTA T = 1.682E+01 TEMP = 120.00
CAP COST = 2.071E+06 HOURLY OP COST = 1.978E+00

REBOILER

QDUT = 2.230E+07 TEMP = 212.57

800PSIA STEAM U=100 DELTA T = 1.254E+02 HOURLY OP COST = 1.115E+01

REBOILER AREA = 1.778E+03 REBOILER CAP COST = 7.655E+03

EQUILIBRIUM STAGES = 31.81 EFFICIENCY = .72862

45 PLATES DIAMETER = 1.070E+0214 PRESSURE = 1.070E+01PSIA TOWER COST = 0.726E+06

TOTAL CAPITAL = 1.155E+09 TOTAL OPERATING = 1.312E+01

YEARLY OPERATING COST IS \$180190.35

SEPARATOR 1 FOR STREAM NUMBER 2
DISTILLATION
LIGHT KEY IS HEXENE

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	7.49983E+02	3.75200E+02	3.74983E+02	
1-PENTENE	.16667	.33333	0.00000	
PENTANE	.16667	.33333	0.00000	
HEXENE	.16667	.33000	.00333	
HEXANE	.16667	.00333	.33001	
BENZENE	.16661	.00000	.33324	
CYCLOHEXANE	.16500	.00000	.33001	
HEPTANE	.00167	.00000	.00333	
TOLUENE	.00004	.00000	.00007	

MINIMUM REFLUX RATIO = 5.16120E+00

CONDENSER

DUTY = 3.406E+07 AREA = 1.156E+04 DELTA T = 1.603E+01 TEMP = 120.00

CAP COST = 3.122E+04 HOURLY OP COST = 3.406E+00

REBOILER

DUTY = 3.710E+07 TEMP = 186.35

EXHAUST STEAM U=150 DELTA T = 3.365E+01 HOURLY OP COST = 9.274E+00

REBOILER AREA = 7.349E+03 REBOILER CAP COST = 2.222E+04

EQUILIBRIUM STAGES = 118.88 EFFICIENCY = .77339

153 PLATES DIAMETER = 1.284E+02 IN PRESSURE = 2.172E+01 PSIA TOWER COST = 6.756E+05
TOTAL CAPITAL = 7.290E+05 TOTAL OPERATING = 1.268E+01

YEARLY OPERATING COST IS \$106513.26

SEPARATOR 3 FOR STREAM NUMBER 4

FOR THE FOLLOWING DISTILLATION 750.000 LB MOLES/HR OF TETRAHYDROFURAN
HAS BEEN ADDED AS AN EXTRACTIVE SOLVENT
DISTILLATION

LIGHT KEY IS PENTANE

HEAVY KEY IS 1-PENTENE

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	1.12500E+03	1.26116E+02	9.98884E+02	
PENTANE	.11210	.98999	.00126	
1-PENTENE	.11216	.01001	.12506	
HEXANE	.00112	.00000	.00127	
HEXENE	.11209	.00000	.12624	
TETRAHYDROFURAN	.66252	.00000	.74617	
BENZENE	.00000	.00000	.00000	

MINIMUM REFLUX RATIO = 1.79310E+01

CONDENSER

DUTY = 3.317E+07 AREA = 1.126E+04 DELTA T = 1.603E+01 TEMP = 120.00

CAP COST = 3.061E+04 HOURLY OP COST = 3.317E+00

REBOILER

DUTY = 3.618E+07 TEMP = 156.13

EXHAUST STEAM U=150 DELTA T = 6.387E+01 HOURLY OP COST = 9.045E+00

REBOILER AREA = 3.776E+03 REBOILER CAP COST = 1.345E+04

EQUILIBRIUM STAGES = 143.35 EFFICIENCY = .76333

160 PLATES DIAMETER = 1.239E+02 IN PRESSURE = 2.256E+01 PSIA TOWER COST = 0.300E+05
TOTAL CAPITAL = 6.749E+05 TOTAL OPERATING = 1.236E+01

YEARLY OPERATING COST IS \$103843.36

SEPARATOR 2 FOR STREAM NUMBER 5

FOR THE FOLLOWING DISTILLATION 749.967 LB MOLES/HR OF PHENOL
HAS BEEN ADDED AS AN EXTRACTIVE SOLVENT

DISTILLATION

LIGHT KEY IS HEXANE

HEAVY KEY IS CYCLOHEXANE

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	1.12495E+03	1.23225E+02	9.99725E+02	
HEXANE	.11000	.97832	.00124	
HEXENE	.00111	.00939	.00007	
HEPTANE	.06111	.00055	.00110	
CYCLOHEXANE	.11002	.00980	.12256	
BENZENE	.11113	.00185	.12482	
TOLUENE	.00002	.00000	.00063	
PHENOL	.66660	.00000	.75010	

MINIMUM REFLUX RATIO = 1.03271E+00

CONDENSER

DUTY = 4.103E+06 AREA = 4.179E+02 DELTA T = 5.610E+01 TEMP = 159.40

CAP COST = 7.588E+03 HOURLY OP COST = 4.103E-01

REBOILER

DUTY = 4.203E+06 TEMP = 222.99

100PSIA STEAM U=100 DELTA T = 1.350E+02 HOURLY OP COST = 2.102E+00

REBOILER AREA = 3.655E+02 REBOILER CAP COST = 2.340E+03

EQUILIBRIUM STAGES = 15.26 EFFICIENCY = .61596

25 PLATES DIAMETER = 4.073E+01IN PRESSURE = 1.470E+01PSIA TOWER COST = 1.908E+04

TOTAL CAPITAL = 2.401E+04 TOTAL OPERATING = 2.512E+00

YEARLY OPERATING COST IS \$ 21100.51

SEPARATOR 2 FOR STREAM NUMBER 7

FOR THE FOLLOWING DISTILLATION 1997.767 LB MOLES/HR OF PHENOL
HAS BEEN ADDED AS AN EXTRACTIVE SOLVENT

DISTILLATION

LIGHT KEY IS HEXENE

HEAVY KEY IS TETRAHYDROFURAN

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	2.99665E+03	2.55537E+02	2.74069E+03	
PENTANE	.00042	.00493	.00000	
1-PENTENE	.04169	.48779	.00002	
HEXANE	.00042	.00493	.00000	
HEXENE	.04208	.48772	.00045	
TETRAHYDROFURAN	.75397	.01663	.27195	
BENZENE	.00000	.00000	.00000	
PHENOL	.66542	.30000	.72756	

MINIMUM REFLUX RATIO = 1.04928E+00

CONDENSER

DUTY = 7.964E+06 AREA = 2.704E+03 DELTA T = 1.683E+01 TEMP = 120.00

CAP COST = 1.050E+04 HOURLY OP COST = 7.964E-01

REBOILER

DUTY = 0.162E+06 TEMP = 228.63

100PSIA STEAM U=100 DELTA T = 1.094E+02 HOURLY OP COST = 4.081E+00

REBOILER AREA = 7.463E+02 REBOILER CAP COST = 3.998E+03

EQUILIBRIUM STAGES = 14.07 EFFICIENCY = .61744

25 PLATES DIAMETER = 6.500E+01IN PRESSURE = 1.930E+01PSIA TOWER COST = 2.847E+04

TOTAL CAPITAL = 4.297E+04 TOTAL OPERATING = 4.077E+00

YEARLY OPERATING COST IS \$ 40569.97

SEPARATOR 1 FOR STREAM NUMBER 9
DISTILLATION

LIGHT KEY IS TOLUENE

HEAVY KEY IS PHENOL

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	9.99725E+02	2.53508E+02	7.46217E+02	
HEXENE	.00007	.00029	.00000	
HEXANE	.00124	.00488	.00000	
BENZENE	.12402	.49200	.00007	
CYCLOHEXANE	.12256	.40327	.00002	
HEPTANE	.00110	.00466	.00000	
TOLUENE	.00003	.00011	.00000	
PHENOL	.75010	.01479	.99991	

MINIMUM REFLUX RATIO = 7.13907E-02

CONDENSER

DUTY = 6.598E+06 AREA = 3.452E+02 DELTA T = 7.612E+01 TEMP = 174.95

CAP COST = 2.242E+03 HOURLY OP COST = 4.598E-01

REBOILER

DUTY = 6.960E+06 TEMP = 358.69

500PSIA STEAM U=60 DELTA T = 1.033E+02 HOURLY OP COST = 4.176E+00

REBOILER AREA = 1.123E+03 REBOILER CAP COST = 5.431E+03

EQUILIBRIUM STAGES = 11.94 EFFICIENCY = .65237

19 PLATES DIAMETER = 5.313E+01IN PRESSURE = 1.470E+01PSIA TOWER COST = 6.09E+04

TOTAL CAPITAL = 2.376E+04 TOTAL OPERATING = 4.636E+00

YEARLY OPERATING COST IS \$ 30942.06

SEPARATOR 1 FOR STREAM NUMBER 11

DISTILLATION

LIGHT KEY IS TETRAHYDROFURAN

HEAVY KEY IS PHENOL

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
	2.74069E+03	7.52909E+02	1.96778E+03	
PENTANE	.00000	.00000	.00000	
1-PENTENE	.00002	.00009	.00000	
HEXANE	.00000	.00001	.00000	
HEXENE	.00006	.00167	.00000	
TETRAHYDROFURAN	.27195	.98599	.00187	
BENZENE	.00000	.00000	.00000	
PHENOL	.72756	.01324	.99013	

MINIMUM REFLUX RATIO = 5.39923E-02

CONDENSER

DUTY = 1.319E+07 AREA = 1.467E+03 DELTA T = 5.136E+01 TEMP = 10.03

CAP COST = 6.637E+03 HOURLY OP COST = 1.319E+03

REBOILER

DUTY = 1.994E+07 TEMP = 356.15

500PSIA STEAM U=60 DELTA T = 1.030E+02 HOURLY OP COST = 1.197E+01

REBOILER AREA = 3.140E+03 REBOILER CAP COST = 1.175E+04

EQUILIBRIUM STAGES = 9.85 EFFICIENCY = .64014

16 PLATES DIAMETER = 9.073E+01IN PRESSURE = 1.470E+01PSIA TOWER COST = 2.975E+04

TOTAL CAPITAL = 4.413E+04 TOTAL OPERATING = 1.328E+01

YEARLY OPERATING COST IS \$111591.51

SEPARATOR 2 FOR STREAM NUMBER 12

FOR THE FOLLOWING DISTILLATION 499.517 LB MOLES/HR OF PHENOL
HAS BEEN ADDED AS AN EXTRACTIVE SOLVENT
DISTILLATION

LIGHT KEY IS CYCLOHEXANE

HEAVY KEY IS BENZENE

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
HEXANE	7.53025E+02	1.25828E+02	6.27998E+02	
HEXENE	.00164	.00998	.00000	
HEPTANE	.00810	.00059	0.00000	
CYCLOHEXANE	.00157	.00945	.00000	
BENZENE	.12269	.97009	.00195	
TOLUENE	.16573	.00998	.19673	
PHENOL	.00004	.00000	.00004	
	.66823	.00000	.60127	

MINIMUM REFLUX RATIO = 4.45311E+00

CONDENSER

DUTY = 1.124E+07 AREA = 8.254E+02 DELTA T = 7.782E+01 TEMP = 176.63

CAP COST = 4.312E+03 HOURLY OP COST = 1.124E+00

REBOILER

DUTY = 1.150E+07 TEMP = 243.82

100PSIA STEAM U=103 DELTA T = 9.418E+01 HOURLY OP COST = 5.748E+00

REBOILER AREA = 1.221E+03 REBOILER CAP COST = 5.782E+03

EQUILIBRIUM STAGES = 46.29 EFFICIENCY = .59812

78 PLATES DIAMETER = 8.037E+01IN PRESSURE = 1.470E+01PSIA TOWER COST = 1.475E+05

TOTAL CAPITAL = 1.576E+05 TOTAL OPERATING = 6.872E+00

YEARLY OPERATING COST IS \$ 57722.67

SEPARATOR 1 FOR STREAM NUMBER 17

DISTILLATION

LIGHT KEY IS TOLUENE

HEAVY KEY IS PHENOL

	FEED	DISTILLATE	BOTTOMS	LB MOLES/HR
BENZENE	6.27998E+02	1.27247E+02	5.00751E+02	
CYCLOHEXANE	.19673	.97038	.00014	
HEPTANE	.00195	.00963	.00000	
TOLUENE	.00000	.00000	.00000	
PHENOL	.00004	.00022	.00000	
	.00127	.01977	.99986	

MINIMUM REFLUX RATIO = 1.14962E-01

CONDENSER

DUTY = 2.437E+06 AREA = 1.781E+02 DELTA T = 7.017E+01 TEMP = 176.98

CAP COST = 1.365E+03 HOURLY OP COST = 2.437E-01

REBOILER

DUTY = 3.835E+06 TEMP = 358.64

500PSIA STEAM U=60 DELTA T = 1.034E+02 HOURLY OP COST = 2.181E+00

REBOILER AREA = 5.861E+02 REBOILER CAP COST = 3.335E+03

EQUILIBRIUM STAGES = 10.92 EFFICIENCY = .64291

17 PLATES DIAMETER = 3.840E+01IN PRESSURE = 1.470E+01PSIA TOWER COST = 9.749E+03

TOTAL CAPITAL = 1.445E+04 TOTAL OPERATING = 2.425E+00

YEARLY OPERATING COST IS \$ 20366.50

STRM	CHPONT	PRODUCT	SEP	NXT	MSA	LST	PRODUCTS IN STREAM																							
MUMB	LE	HK	HK	LK	NUM	STR	RCL	STR	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2
1	3	2	1	2	3	2	22	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	8	9	0	1	2
2	4	5	4	2	8	4	8	1	2	3	4	5	6	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	17	1	1	7	1	6	0	1	1	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	1	3	2	14	1	8	0	2	2	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	8	5	4	5	6	10	18	2	3	4	5	6	9	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	3	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	4	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	8	9	6	5	2	12	16	5	5	6	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	5	6	3	4	7	14	20	5	3	4	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	11	8	5	8	1	16	0	10	5	8	0	0	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	18	9	6	12	1	18	10	6	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	16	5	4	13	1	20	0	11	4	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	12	6	3	9	1	22	0	11	3	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	12	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	12	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	13	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	13	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	14	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	15	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	15	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

SEPARATOR 3 FOR STREAM NUMBER 1

TWO SECTION EXTRACTION
LIGHT KEY IS PR

	FEED	HEAVY KEY	IS CE	EXTRACT	RAFFINATE	LBH/HR
	3.00000	12.18667	45.44444	12.18614	45.44442	
TOP2.9KHN03	0.00000	1.00000	0.00000	.99802	.00099	
GD	.00013	0.00000	0.00000	.00003	.00001	
EU	.00002	0.00000	0.00000	.00001	.00000	
TO	.00002	0.00000	0.00000	.00001	.00000	
DY	.00002	0.00000	0.00000	.00001	.00000	
SH	.00053	0.00000	0.00000	.00013	.00000	
ND	.30486	3.00000	0.00333	.00120	.00300	
PR	.00150	0.00000	0.00000	.00035	.00000	
GE	.01175	0.01000	0.00500	.00014	.00369	
LA	.00614	0.00000	0.00000	.00000	.00038	
WATER	.97506	0.00000	1.00000	.00010	.99793	

SURFACE TENSIONS = 6.81730E+01 9.75339E+01
 EFFICIENCY = .326 DENSITY DIFFERENCE (LBH/FT3) = 127.779
 SURFACE TENSIONS = 6.92121E+01 5.72123E+01
 EFFICIENCY = .300 DENSITY DIFFERENCE (LBH/FT3) = 126.613
 SECTION A PLATES = 109 DIAMETER(IN) = 6.46
 SECTION B PLATES = 124 DIAMETER(IN) = 6.46
 TOTAL CAPITAL COST = 2.00921E+04
 TEMP(F) = 100.000

SEPARATOR 8 FOR STREAM NUMBER 2
TWO SECTION EXTRACTION
LIGHT KEY IS ND

	FEED	SOLVENT	HEAVY KEY IS SM REFLUXER	EXTRACT	RAFFINATE	LBMOLES/HR
12.5MMNO3H2OVSTBP	12.15614 0.00000	140.80461 1.00000	14.57323 0.00000	140.81489 .99974	26.71921 .00099	
WATER	.00010	0.00000	0.00000	.00001	.00000	
CE	.00014	0.00000	0.00000	.00001	.00000	
PR	.00035	0.00000	0.00000	.00003	.00000	
NO	.00120	0.00000	0.00000	.00010	.00003	
SM	.00013	0.00000	0.00000	.00000	.00006	
EU	.00001	0.00000	0.00000	.00000	.00000	
GD	.00003	0.00000	0.00000	.00000	.00001	
TB	.00001	0.00000	0.00000	.00000	.00000	
DY	.00001	0.00000	0.00000	.00000	.00000	
TBP2.9MMNO3	.99602	0.00000	1.00000	.00011	.99890	

SURFACE TENSIONS = 5.72123E+01 6.93339E+01
EFFICIENCY = .233 DENSITY DIFFERENCE (LBH/FT3) = 128.349
SURFACE TENSIONS = 5.72732E+01 6.92086E+01
EFFICIENCY = .305 DENSITY DIFFERENCE (LBH/FT3) = 128.297
SECTION A PLATES = 16 DIAMETER(IN) = 9.22
SECTION B PLATES = 32 DIAMETER(IN) = 9.24
TOTAL CAPITAL COST = 4.97591E+03
TEMP(F) = 100.000

SEPARATOR 1 FOR STREAM NUMBER 3
NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.4700E+01
PRESSURE IN DRUM = 2.90747E-26 PSIA
FLASH DRUM WITH BOILER

LIGHT KEY IS WATER

HEAVY KEY IS LA

REBOILER

DUTY = 6.842E+04 TEMP = 100.00
EXHAUST STEAM U=150 DELTA T = 1.200E+02 HOURLY OP COST = 1.210E-02
REBOILER AREA = 2.690E+00 REBOILER CAP COST = 5.881E+01
FEED VAPOR LIQUID
4.84684E+01 4.84176E+01 5.07963E-02 LB MOLES/HR
WATER .99793 .99898 .00000
TBP2.9MMNO3 .00099 .00099 .00000
PR .00000 .00000 .00003
ND .00000 .00000 .00000
LA .00036 .00002 .34449
CE .00069 .00000 .65548

SEPARATOR 1 FOR STREAM NUMBER 4
NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.4700E+01
PRESSURE IN DRUM = 4.03312E-22 PSIA
FLASH DRUM WITH BOILER

LIGHT KEY IS 12.5MMNO3H2OVSTBP

HEAVY KEY IS PR

REBOILER

DUTY = 1.408E+05 TEMP = 100.00
EXHAUST STEAM U=150 DELTA T = 1.200E+02 HOURLY OP COST = 3.520E-02
REBOILER AREA = 7.822E+00 REBOILER CAP COST = 1.310E+02
FEED VAPOR LIQUID
1.40815E+02 1.40795E+02 1.95898E-02 LB MOLES/HR
WATER .00001 .00001 .00000
12.5MMNO3H2OVSTBP .99974 .99988 .00000
TBP2.9MMNO3 .00013 .00011 .00000
EU .00000 .00000 .00000
SM .00000 .00000 .00000
GD .00000 .00000 .00000
PR .00003 .00000 .20532
ND .00010 .00000 .70513
CE .00001 .00000 .00000

SEPARATOR 6 FOR STREAM NUMBER 5
TWO SECTION EXTRACTION
LIGHT KEY IS T3

	FEED	SOLVENT	HEAVY KEY IS SM REFLUXER	EXTRACT	RAFFINATE	LBMOL/HR
	26.71921	86.73174	183.78141	86.95971	210.67265	
	0.00000	1.00000	0.00000	.99999	.00001	
.266MHN03H2OVSTBP						
12.5MHN03H2OVSTBP	.00099	0.00000	0.00000	.00031	.00003	
OY	.00010	0.00000	0.00000	.00000	.00000	
CE	.00000	0.00000	0.00000	.00000	.00000	
TD	.30440	0.00000	0.00000	.00000	.00000	
PR	.00000	0.00000	0.00000	.00000	.00000	
ND	.33023	0.00000	0.00000	.00000	.00000	
SM	.00000	0.00000	0.00000	.00000	.00000	
GD	.00001	0.00000	0.00000	.00000	.00000	
EU	.00000	0.00000	0.00000	.00000	.00000	
TBP2.9MHN03	.99890	0.00000	1.00000	.00011	.99989	

SURFACE TENSIONS = 5.72123E+01 6.84386E+01
EFFICIENCY = .130 DENSITY DIFFERENCE(LBM/FT3) = 128.658
SURFACE TENSIONS = 5.72639E+01 6.84303E+01
EFFICIENCY = .123 DENSITY DIFFERENCE(LBM/FT3) = 128.691
SECTION A PLATES = 123 DIAMETER(IN) = 20.22
SECTION B PLATES = 144 DIAMETER(IN) = 21.51
TOTAL CAPITAL COST = 1.34460E+05
TEMP(F) = 100.000

SEPARATOR 2 FOR STREAM NUMBER 10
PH CHANGE 20.25 LBMOL/HR OF NASH ADDED AT COST OF \$ 2.03E+02

TWO SECTION EXTRACTION
LIGHT KEY IS T8

	FEED	SOLVENT	HEAVY KEY IS OY REFLUXER	EXTRACT	RAFFINATE	LBMOL/HR
	106.81468	3571.82019	1061.43995	3570.69749	1169.37733	
	0.33300	1.00000	0.00000	.99999	.00001	
TBP.266MHN03						
TBP2.9MHN03	.00009	0.00000	0.00000	.00000	.00000	
EU	.00000	0.00000	0.00000	.00000	.00000	
GD	.00000	0.00000	0.00000	.00000	.00000	
SH	.00000	0.00000	0.00000	.00000	.00000	
ND	.00000	0.00000	0.00000	.00000	.00000	
PR	.00000	0.00000	0.00000	.00000	.00000	
TD	.30440	0.00000	0.00000	.00000	.00000	
CE	.00000	0.00000	0.00000	.00000	.00000	
OY	.00440	0.00000	0.00000	.00000	.00000	
12.5MHN03H2OVSTBP	.00025	0.00000	0.00000	.00000	.00000	
WATER	.18963	0.00000	0.00000	.00000	.00000	
.266MHN03H2OVSTBP	.81003	0.00000	1.00000	.00001	.99999	

SURFACE TENSIONS = 6.84333E+01 5.69835E+01
EFFICIENCY = .105 DENSITY DIFFERENCE(LBM/FT3) = 128.207
SURFACE TENSIONS = 6.84725E+01 5.69830E+01
EFFICIENCY = .109 DENSITY DIFFERENCE(LBM/FT3) = 127.610
SECTION A PLATES = 366 DIAMETER(IN) = 82.74
SECTION B PLATES = 230 DIAMETER(IN) = 82.76
TOTAL CAPITAL COST = 1.47837E+06
TEMP(F) = 100.000

SEPARATOR 7 FOR STREAM NUMBER 11
TWO SECTION EXTRACTION
LIGHT KEY IS SM

	FEED	SOLVENT	HEAVY KEY IS EU REFLUXER	EXTRACT	RAFFINATE	LB MOLES/HR
2.9MHN03H2OVSTBP	210.67265	3553E+0000	4959.67476	35526.01735	5179.22062	
	0.00000	1.00000	0.00000	.99999	.00000	
.266MHN03H2OVSTBP	.00099	0.00000	0.00000	.00001	.00000	
PR	.00000	0.00000	0.00000	.00000	.00000	
ND	.00000	0.00000	0.00000	.00000	.00000	
SM	.00001	0.00000	0.00000	.00000	.00000	
DY	.00000	0.00000	0.00000	.00000	.00000	
YB	.00000	0.00000	0.00000	.00000	.00000	
EU	.00000	0.00000	0.00000	.00000	.00000	
GD	.00000	0.00000	0.00000	.00000	.00000	
TBP2.9MHN03	.99900	0.00000	1.00000	.00000	.99900	

SURFACE TENSIONS = 5.72123E+01 6.86807E+01
EFFICIENCY = .279 DENSITY DIFFERENCE (LBH/FT3) = 128.605
SURFACE TENSIONS = 3.72598E+01 6.86866E+01
EFFICIENCY = .285 DENSITY DIFFERENCE (LBH/FT3) = 128.578
SECTION A PLATES = 19# DIAETER (IN) = 12.02
SECTION B PLATES = 200 DIAMETER (IN) = 120.06
TOTAL CAPITAL COST = 1.67986E+06
TEMP (F) = 100.000

SEPARATOR 1 FOR STREAM NUMBER 12
NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.4700E+01
PRESSURE IN DRUM = 2.96213E-13 PSIA
FLASH DRUM WITH BOILER

LIGHT KEY IS TBP.266MHN03

HEAVY KEY IS TB

REBOILER

DUTY = 3.571E+06 TEMP = 100.00
EXHAUST STEAM U=15# DELTA T = 1.260E+02 HOURLY OP COST = 8.927E-01
REBOILER AREA = 1.984E+02 REBOILER CAP COST = 1.480E+03
FEED VAPOR LIQUID
3.57670E+03 3.57470E+03 2.2119E+04 LB MOLES/HR
.266MHN03H2OVSTBP .00001 .00000 .00000
TBP.266MHN03 .99999 .99999 .00000
TBP2.9MHN03 .00000 .00000 .00000
EU .00000 .00000 .00000
SM .00000 .00000 .00000
DY .00000 .00000 .00000
TB .00000 .00000 .00000
GD .00000 .00000 .00000
PR .00000 .00000 .00000
ND .00000 .00000 .00000

SEPARATOR 1 FOR STREAM NUMBER 13
NONCONVERGENCE IN VLQ TEMP = 450.000 PRESSURE = 1.4700E+01
PRESSURE IN DRUM = 1.11851E-11 PSIA
FLASH DRUM WITH BOILER

LIGHT KEY IS .266MHN03H2OVSTBP

HEAVY KEY IS DY

REBOILER

DUTY = 1.169E+06 TEMP = 100.00
EXHAUST STEAM U=15# DELTA T = 1.260E+02 HOURLY OP COST = 2.923E-01
REBOILER AREA = 6.497E+01 REBOILER CAP COST = 6.407E+02
FEED VAPOR LIQUID
1.16938E+03 1.16938E+03 7.5818E+05 LB MOLES/HR
HATCO .00000 .00000 .00000
.266MHN03H2OVSTBP .98166 .98166 .00000
12.5MHN03H2OVSTBP .00000 .00000 .00000
TBP.266MHN03 .00164 .00164 .00000
DY .00000 .00000 .94949
TB .00000 .00000 .04675
PR .00000 .00000 .00376

STREAM NUMBER	1	2	3	4	5	6	7	8	9	10
FEED RATE	3.00	12.2	40.5	141	26.6	48.6	5.080E-02	141	1.959E-02	86.6
TEMPERATURE (F)	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
PRESSURE (PSIA)	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700
STATE	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	VAPOR	LIQUID	LIQUID
LA	.6140E-02	.6240E-11	.3000E-03	0.	0.	.1902E-06	.3445E+00	0.	0.	0.
CE	.1175E-01	.1443E-03	.6911E-03	.1266E-04	.1379E-07	.4128E-05	.6555E+00	.3444E-10	.8954E-01	.2628E-06
PN	.1711E-12	.3916E-13	.6661E-15	.3317E-16	.1517E-15	.4634E-05	.3421E-04	.1504E-05	.2033E+00	.1382E-06
NO	.4100E-02	.1204E-02	.2163E-07	.9874E-04	.2749E-04	.2040E-07	.1127E-05	.6476E-06	.7051E+00	.1092E-05
SH	.6303E-03	.1300E-03	.2284E-12	.5605E-06	.6595E-04	0.	0.	.5606E-06	.4594E-14	.7036E-06
EU	.7500E-04	.6173E-05	.1063E-15	.2858E-18	.2792E-05	0.	0.	.2858E-18	.1118E-18	.7562E-08
GO	.1250E-03	.3065E-04	.2815E-15	.3925E-04	.1431E-34	0.	0.	.3431E-08	.3553E-05	.5457E-07
TO	.2500E-04	.6173E-05	.2247E-15	.2302E-10	.2307E-05	0.	0.	0.	0.	.6669E-06
OY	.2500E-04	.6173E-05	.1519E-13	.4368E-11	.2897E-05	0.	0.	0.	0.	.7116E-16
WATER	.975E+00	.9979E+00	.9996E+00	.1100E-03	.9989E+00	.9991E+00	.1650E-20	.0651E-05	.3242E-29	.1895E-16
TDP2.9MHND3	0.	.9900E+00	.9906E-02	0.	.9999E+00	.9991E+00	.5132E-29	.1112E-03	.1487E-25	.0032E-04
.266MHND3H2OVS	0.	0.	0.	0.	0.	0.	0.	0.	0.	.6100E+03
12.5MHND3H2OVS	0.	0.	0.	0.	.9997E+00	.9995E+00	0.	.9999E+00	.2444E-24	.2478E-03

STREAM NUMBER	11	12	13	14	15	16	17	18	19	20
FEED RATE	211	3.671E+03	1.169E+03	3.553E+04	5.175E+03	3.571E+03	2.211E-04	1.169E+03	7.582E-05	3.593E+04
TEMPERATURE (F)	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000	100.000
PRESSURE (PSIA)	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700	14.700
STATE	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	VAPOR	LIQUID	VAPOR
CE	.1617E-11	.6936E-18	.2823E-11	0.	0.	0.	0.	0.	0.	0.
PN	.2908E-07	.9440E-08	.2435E-09	.1676E-09	.1498E-20	.2309E-14	.1524E+00	.1543E-17	.3762E-02	.1526E-23
NO	.2931E-05	.3266E-07	.2704E-11	.1739E-07	.6780E-14	.1036E-14	.5275E+00	0.	0.	.9765E-22
SH	.6816E-05	.2145E-07	.2047E-12	.3839E-07	.1391E-17	.2195E-07	.3253E-17	0.	0.	.1920E-08
EU	.7503E-06	.2622E-09	.1627E-15	.1035E-09	.1335E-07	.2262E-09	.4245E-11	0.	0.	.3591E-10
GO	.1750E-05	.1633E-08	.2197E-14	.2150E-09	.6975E-07	.4946E-13	.2636E-01	0.	0.	.9919E-22
TO	.1787E-07	.1856E-07	.3634E-03	.1284E-10	.6391E-09	.9478E-19	.2948E+04	.2738E-11	.4675E-01	0.
OY	.1674E-09	.6219E-09	.6282E-07	.9396E-12	.3637E-12	.2308E-09	.2957E-02	.1255E-08	.9495E+00	0.
WATER	0.	.3742E-17	.1732E-01	0.	0.	0.	0.	.1732E-01	.7387E-16	0.
TDP2.9MHND3	0.	.1000E+01	.9990E-03	0.	0.	.1000E+01	.7914E-13	.9996E-03	.6233E-14	0.
TDP2.9MHND3	.999E+01	.2672E-25	.1424E-10	.1000E-05	.9190E+00	.2672E-05	.2145E-18	0.	0.	.1000E-05
.266MHND3H2OVS	.9993E-03	.1000E-04	.9817E+00	.5867E-05	.5149E-18	.1000E-04	.1112E-20	.9817E+00	.4117E-14	.5867E-05
2.9MHND3H2OVS	0.	0.	.1000E+01	.9892E-03	0.	0.	0.	0.	0.	.1000E+01
12.5MHND3H2OVS	.2134E-17	.2929E-116	.2263E-04	0.	0.	0.	0.	.2263E-04	.9317E-19	0.

STREAM NUMBER	21	22	23	24	25	26	27	28	29	30
FEED RATE	1.928E-03	5.175E+03	5.033E-04	0.	0.	0.	0.	0.	0.	0.
TEMPERATURE (F)	100.000	100.000	100.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRESSURE (PSIA)	14.700	14.700	14.700	0.000	0.000	0.000	0.000	0.000	0.000	0.000
STATE	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
PR	.3257E-02	0.	0.	0.	0.	0.	0.	0.	0.	0.
NO	.3205E+00	0.	0.	0.	0.	0.	0.	0.	0.	0.
SH	.6722E+06	.3071E-11	.1430E+00	0.	0.	0.	0.	0.	0.	0.
EU	.1410E-03	.6774E-09	.1322E+00	0.	0.	0.	0.	0.	0.	0.
GO	.3962E-02	.1006E-20	.7122E+00	0.	0.	0.	0.	0.	0.	0.
TO	0.	.1993E-20	.6571E-02	0.	0.	0.	0.	0.	0.	0.
TDP2.9MHND3	.7.59E-11	.9994E+00	.0371E+03	0.	0.	0.	0.	0.	0.	0.
.266MHND3H2OVS	.6477E-13	0.	0.	0.	0.	0.	0.	0.	0.	0.
2.9MHND3H2OVS	.7512E-08	.9892E-03	.9005E-09	0.	0.	0.	0.	0.	0.	0.

APPENDIX D

Individual Separator Simulations

Distillation

Simulation of the distillation unit is the most complex in terms of the heuristics used. The formal parameters for input are (1) identification of the light and heavy key components and their split fraction into the distillate and bottoms, respectively; (2) the thermal condition and temperature of the feed; and (3) the maximum allowable temperature in the bottom. Through common storage feed rate, feed composition, and thermodynamic parameters pass. Routine DISTL controls the simulation.

The minimum number of stages is calculated by FRAC using the Fenske-Underwood Equation. The relative volatilities are calculated based on the activity coefficients of the components at the feed composition and the temperature of the feed, or at 130°F if a pressurized column is used. Based on the total-reflux equations the splits of all of the components are calculated by routine FRAC2. If the minimum number of stages is less than one, routine VLQ attempts to make the separation in a flash drum or partial condenser. It does this by trying to find the temperature and pressure at which the specified split fractions of the keys are exactly met, if they are not satisfied, or by dividing the improvement in the split fractions if they are more than met. If VLQ fails, the next step is to use a distillation column. The minimum reflux is calculated using the Underwood equations (King, 1971). This calculation is also iterative. The operating reflux is set at 1.3 times the minimum rate, which is a heuristic.

At first the column is set to atmospheric pressure. If the bubble point (by BUBL) of the distillate is greater than 120°F , so that cooling water can be used in the overhead condenser, then the bubble point and the latent heat (both by BUBL) of the bottoms are calculated. If the maximum allowable temperature (usually 600°F) is not exceeded, the reboiler is sized and costed by RBL. If the maximum temperature is exceeded, a vacuum tower is tried at a reboiler temperature equal to the maximum allowable and a corresponding pressure. Allowing for a pressure drop of one inch of water on each tray, the overhead pressure must be attainable with a one-stage steam ejector, i.e., 1.5 psia. If this is not possible, distillation is not used and a constraint is considered violated. If the distillate bubble point is less than 120°F , a pressure column is used in order to increase the overhead temperature so that cooling water can be used, if possible. If this cannot be done without increasing the pressure beyond 60% of the critical pressure of the mixing, cooling water is not used. Above 50°F steam ejectors provide low-pressure evaporation of water, and below that refrigeration is used at several discrete levels. Capital costs are included for these coolants. If the pressure exceeds 115 psia a partial condenser is used, and the distillate is taken as a vapor product.

Increased pressure increases the cost of the tower, the basic cost of which is taken from a graph in Peters and Timmerhaus (p. 659). The cost of plates in excess of 50 is double the normal cost. The actual number of ideal stages is taken from the Gilliland correlation (Perry, 1963). The efficiency is based on a correlation in Maxwell (1950). The viscosity is obtained through the method of Stiel and Thodos (Ried and Sherwood, 1966):
$$\text{eff} = 36.3 (\text{vis}, \text{cp})^{.46}$$

Extractive Distillation

Extractive distillation is simulated in the same way as distillation except that the solvent is added to the extent of 67% mole percent of the total liquid feed. The bottoms composition is also checked by routine MISBL to assure that it corresponds to one homogeneous phase. No direct charge of capital or make-up is made for the solvent.

Extraction

Single-section extraction simulation is based on the Kremser-Souders-Brown equation (King, 1971) in routine EXTOR. The stripping factor is set at 1.40. Distribution coefficients are calculated based on the activity coefficients of the actual feed phase and the limiting activity coefficients at high dilution in the solvent phase. Only the light key and its split fraction are identified. The internal countercurrent flow ratio is checked to see if it exceeds 10 to one (i.e., within the distribution coefficient of the light key lies outside the range: 0.14 to 14.0). If it does violate the constraint, the temperature is changed until the ratio falls within the proper range, or until the temperature goes outside the range between the solvent bubble point and -200°F . Low-temperature operation is charged additional capital costs in discrete levels for the materials used. Plates in excess of 50 are costed at double the normal price. The unit is sized by routine SXX. It follows the example in Treybal (1963), p. 378, using sieve plates with a hole size of $3/16''$ on a $3/4''$ triangular spacing and a maximum velocity through the holes of 0.7 ft/sec. The efficiency is from Treybal (1963), p. 507. The densities are calculated from the correlation given by Halm and Thodos (1970). The

interfacial tension is taken to be the difference between the surface tensions of the two fluids (Reid and Sherwood, 1966). The surface tension is calculated from corresponding states (Reid and Sherwood, 1966).

Two-section extraction incorporates everything that is simulated in the single-section, except that both key components must be considered. The two solvent flow rates are established by setting the stripping factors in each section equal, in one section using the distribution coefficient of the light key and in the other, that of the heavy key. The calculation is made more difficult because a stream must be cut, each section calculated separately, and both sides of the cut stream must match. This iterative calculation requires more time and makes the programming more difficult, but the concepts are the same as for the single section. Both sections are sized by SXX.

Stripping

Stripping is simulated as single-section extraction except for the calculation of the distribution coefficients and the sizing. The distribution coefficients are based on the actual activity coefficients in the liquid feed stream. The unit is sized by routine SSA. A sieve plate column is used. The sizing is done as in King, Chapter 12 (1971). The same efficiency correlation as for distillation is used.

Absorption

The absorption unit simulator is also similar to the extraction unit. The Kremser Equation uses the distribution of the heavy key instead

of that of the light key. The absorption factor is set at 0.7 and only the split fraction of the heavy key is used. The sizing is done by routine SSA.

An absorber-stripper is simulated as a two-section extractor, except for the distribution coefficients and sizing by SSA.

Utility Costs

The cost of utilities is as given in Peters and Timmerhaus (1968) p. 776. Water is \$ 0.02/1000 gal., electricity is \$ 0.01/kwhr, 500 psia steam is \$ 0.60/1000 lb, 100 psia steam is \$ 0.50/1000 lb, and exhaust steam is \$ 0.25/1000 lb. These utility costs are used as the operating costs in the economic evaluation. Postulating about a four year pay-out, the purchased cost of equipment (which represents about one-fourth of the installed cost) is added to operating cost for one year's operation. This combined cost is used as the economic criterion in the synthesis.

Appendix E

Immiscibility in Liquid Systems

This appendix discusses three tests for partial immiscibility which were developed for use in checking the homogeneity of a liquid mixture in simulating separation processes. The three tests are programmed sequentially, in order of increasing complexity. Positive results on any one of them are sufficient to establish that the mixture tested does not form a single, stable liquid phase. Unfortunately, negative results on all three tests do not guarantee homogeneity of the mixture, but the region of uncertainty is rather small. If all the tests fail, homogeneity is assumed.

The tests are discussed and implemented separately for two ternary systems. Although the Gibbs energy in the synthesizer program is based on calculations for regular solution theory, the tests are illustrated with examples that employ the NRTL equations because the parameters and the experimental data were known for these systems (Renon, 1971).

At a given temperature and pressure, a multicomponent mixture forms more than one phase if, by doing so, the total Gibbs energy of the system can be decreased relative to that of the single phase.

The Gibbs energy of a system having any number of phases can be divided into two parts -- a contribution from the Gibbs energy of mixing and a contribution from the Gibbs energy of the pure components.

$$G_{\text{system}} \equiv \frac{G_{\text{system}}}{n_T}$$

$$G_{\text{system}} = \sum_l^{\pi} G_l$$

where

$$G_l = \sum_i^N (n_{il} \varepsilon_i^{\text{pure}}) + \sum_i^N n_{il} \varepsilon_l^m$$

by noting

$$x_i = \sum_l^{\pi} n_{il} / n_T$$

and defining

$$\alpha_l \equiv \sum_i^N n_{il} / n_T$$

then

$$G_{\text{system}} = \frac{\sum_l^{\pi} G_{\text{system}}}{n_T} = \sum_l^{\pi} \sum_i^N \frac{n_{il}}{n_T} \varepsilon_i^{\text{pure}} + \sum_l^{\pi} \sum_i^N \frac{n_{il}}{n_T} \varepsilon_l^m$$

or

$$G_{\text{system}} = \sum_i^N x_i \varepsilon_i^{\text{pure}} + \sum_l^{\pi} \alpha_l \varepsilon_l^m \quad (1)$$

For a given mixture to be tested, the first term in Eq. (1) is a constant, independent of the number of phases present at equilibrium. Hence, only the second term - the Gibbs energy of mixing - need be examined to establish if the Gibbs energy of the system is at a minimum or not. Positive results to any of the three non-iterative tests described below establish that the Gibbs energy of the system is not at a minimum, and hence the system is heterogeneous.

Test No. 1 - The function g^m , assuming homogeneity

If the Gibbs energy of mixing for the mixture to be tested (considering the mixture as a single homogeneous phase) is greater than zero, clearly the mixture is immiscible since, if nothing else, pure components can be split out as additional phases. The g^m for a phase of a pure component is zero by definition (see Eq. (1)). The Gibbs energy of mixing can thus be decreased at least to a zero value. The first test is then:

$$g^m > 0 \quad (2)$$

Test No. 2 - The first derivative of the function g^m , assuming homogeneity

The concept of spitting out phases of pure components that is discussed under Test No. 1 can be generalized to be useful even if g^m is less than zero. If the gradient of the Gibbs-energy-of-mixing function (assuming the system to be a single phase) is such that its extrapolation in the direction of a pure component i to $x_i = 1$ would result in $g^m > 0$, then the g^m of the mixture being tested can be decreased by splitting out a new phase of pure component i . The gradient that is desired is the logarithm of the activity of the component in the assumed homogeneous phase. Consider the following:

If g^m of the system is negative and the extrapolated g^m at $x_i = 1$ is positive, then the gradient in question, $RT \ln a_i$, is positive. Creating a new phase of pure component i in a small amount δ would result in a total molar Gibbs energy of mixing for the system of

$$G^m = \delta (g^m)_{x_i=1} + (1 - \delta) (g^m - \delta RT \ln a_i)_{x=y} \quad (3)$$

where y is the composition of the mixture to be tested, and a_i is the

activity of component i.

Since $(g^m)_{x_i=1}$ is zero, the g^m calculated by Eq. (3) is less than $g^m_{x=y}$ if the gradient term is positive. Therefore, the Gibbs energy of mixing at the initial composition $(g^m_{x=y})$ is not the minimum value for the system and the mixture is heterogeneous. This gradient test is made at the point to be tested in the direction of each of the N components in the mixture. A positive result for this test for any component establishes heterogeneity. The gradient that is desired, $RT \ln a_i$, can be calculated from g^m :

$$\begin{aligned}
 n_T dg &= dn_T g - g \sum_i^N dn_i = \sum_i^N \left(\frac{\partial g}{\partial x_i} \right) (dn_i - x_i \sum_k^N dn_k) \\
 dn_T g &= \sum_i \left(\frac{\partial g}{\partial x_i} \right)_{x_{\neq i}} dn_i + \left(g - \sum_i^N \left(\frac{\partial g}{\partial x_i} \right)_{x_{\neq i}} x_i \right) \sum_k^N dn_k \\
 \left(\frac{\partial n_T g}{\partial n_j} \right)_{n_{\neq j}} &= \left(\frac{\partial g}{\partial x_j} \right)_{x_{\neq j}} + \sum_{i \neq j}^N \left(\frac{\partial g}{\partial x_i} \right) \left(\frac{\partial n_i}{\partial n_j} \right)_{n_{\neq j}} \\
 &\quad + \left(g - \sum_i^N x_i \left(\frac{\partial g}{\partial x_i} \right)_{x_{\neq i}} \right) \sum_k^N \left(\frac{\partial n_k}{\partial n_j} \right)_{n_{\neq j}} \\
 RT \ln a_i &= \left(\frac{\partial n_T g^m}{\partial n_i} \right)_{n_j} = \left(\frac{\partial g^m}{\partial x_i} \right)_{x_{\neq i}} + g^m - \sum_k^N x_k \left(\frac{\partial g^m}{\partial x_k} \right)_{x_{\neq k}} \quad (4)
 \end{aligned}$$

where

n is the number of moles and n_T is the total number of moles.

The second test is then:

$$g_{x=y}^m + (1 - y_1)(RT \ln a_1) > 0 \quad (5)$$

for any $i = 1, 2, \dots, N$.

Test No. 3 - Evaluation of second derivatives of the function g^m

Unlike Test No. 2, the criterion for this third test is well-known for a binary system (Prausnitz, 1969). For a multicomponent system, the criteria are also known, but they are more obscure and are quoted in only a few books, e.g., Haase (1956). Test No. 3 checks for a region that, in 2- or 3-dimensional space, could be called "concave downward". Consider the binary system in Fig. 1. Region a is concave downward and is sometimes termed the unstable region. Regions b' and B'' are called metastable. All three regions correspond to compositions that are physically unreal at equilibrium; a liquid mixture whose overall composition is in this region separates into two liquid phases with compositions x' and x'' . Clearly, there are compositions in the unstable region which would not be found to be immiscible by Test No. 1 or Test No. 2 e.g., Region c in Fig. E-1. Test No. 3 can correctly evaluate all compositions for a multicomponent system in the unstable region as heterogeneous, but will not identify conditions in the metastable region.

For a system of N components, a necessary and sufficient condition for having a composition ($\underline{x} \equiv x_1, x_2, x_3, \dots, x_N$) in the unstable region is

$$\Delta_g^2(\underline{x}) \equiv 1/2 \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \left(\frac{\partial^2 g^m(\underline{x})}{\partial x_i \partial x_j} \right) \Delta x_i \Delta x_j < 0 \quad (6)$$

where Δx is some small change in the mole fraction from $\underline{x}$.

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Fig. B-1. Binary free energy curve for partially miscible system.

Since in an N-component system only N-1 mole fractions can be considered independent variables, the N th component is arbitrarily taken here as dependent. In Eq. (6) the derivative requires that temperature, pressure, and all mole fractions except x_N and x_k be held constant (where the derivative is with respect to x_k). The double summation term in Eq. (6) is called a quadratic form and can be equivalently rewritten as the product of three matrices, where the first matrix is the transpose of the third (i.e., a column vector Δx):

$$\sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \left(\frac{\partial^2 g^m}{\partial x_i \partial x_j} \right) \Delta x_i \Delta x_j = [\Delta x_1 \ \Delta x_2 \ \dots \Delta x_{N-1}] \begin{bmatrix} \frac{\partial^2 g^m}{\partial x_1^2} & \dots & \frac{\partial^2 g^m}{\partial x_1 \partial x_{N-1}} \\ & & \vdots \\ \frac{\partial^2 g^m}{\partial x_2 \partial x_1} & & \vdots \\ & & \vdots \\ & & \frac{\partial^2 g^m}{\partial x_{N-1} \partial x_1} & \frac{\partial^2 g^m}{\partial x_{N-1}^2} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \vdots \\ \Delta x_{N-1} \end{bmatrix} \quad (7)$$

A mathematical property of this quadratic form of particular interest here is that the product of the matrices is always a positive scalar quantity for all possible variations of Δx (except the trivial $\Delta x = 0$) if and only if the symmetric matrix of the second derivatives is positive definite (Korn and Korn, 1968, p. 416). This implies that to determine if a particular composition of a liquid system is in the unstable region, possible variations in mole fractions of the components in the system (Δx) that appear in Eq. (6) can be ignored, and only the one matrix of derivatives need be tested for positive definiteness. If the matrix is not positive definite, Eq. (6) is satisfied and the composition being

tested has been found to be immiscible by Test No. 3.

Testing for positive definiteness for a system with many components can be computationally time-consuming. One simple test for positive definiteness requires that all determinants, composed of elements beginning in the upper left-hand corner of the matrix and increasing in size, be positive. That is to say, $\det[e_{11}]$ and $\det \begin{bmatrix} e_{11} & e_{12} \\ e_{21} & e_{22} \end{bmatrix}$ and ... and $\det[(\text{entire matrix})]$ must be positive for the matrix to be positive definite. For a binary system this test is given by the familiar equation

$$\left(\frac{\partial^2 G^m}{\partial x_1^2} \right) > 0 \quad (8)$$

For a ternary system the necessary conditions are Eq. (8) and Eq. (9).

$$\left(\frac{\partial^2 G^m}{\partial x_1^2} \right) \left(\frac{\partial^2 G^m}{\partial x_2^2} \right) - \left(\frac{\partial^2 G^m}{\partial x_1 \partial x_2} \right)^2 > 0 \quad (9)$$

The evaluation of all of the determinants directly is computationally cumbersome. A wholly equivalent test criterion for positive definiteness involves transforming the matrix into row-eshelon form by pivoting, beginning with the upper left-hand element and working systematically downward. The mathematical algorithm used in this transformation is Gaussian elimination as modified by Cholesky to take advantage of the symmetry of the matrix (Korn and Korn, 1968, p. 730). If all of the pivots employed in this manipulation are positive, then the matrix is positive definite (Noble, 1969). Computation need only proceed until a negative pivot is encountered, indicating that the matrix is not positive definite (and hence establishing that the mixture is heterogeneous). The

recursion formulae for this method of pivoting are as follows:

$$\begin{aligned} p_{i1} &= e_{i1} \quad (i = 1, 2, \dots, N-1) \\ p_{ik} &= e_{ik} - \sum_{j=1}^{N-1} \frac{p_{ij} p_{kj}}{p_{jj}} \quad e \quad (i, k = 2, 3, \dots, N-1; i \geq k) \end{aligned} \quad (10)$$

where p_{ij} are the transformed elements,

p_{mm} ($m = 1, 2, \dots, N-1$) are the pivot elements, and

$p_{mm} \leq 0$ (for any m) implies that the matrix is not positive definite.

Examples

Two examples are given here to illustrate the utility of the combined three tests. Two ternary mixtures are considered and the NRTL equation is used to represent the excess Gibbs energy (Prausnitz, 1969, p. 250):

$$\frac{E}{RT} = \sum_{i=1}^{N=3} \left(x_i \frac{\sum_{j=1}^{N=3} x_j G_{ji} \tau_{ji}}{\sum_{k=1}^{N=3} x_k G_{ki}} \right) \quad (11)$$

The molar Gibbs energy of mixing is related to the excess Gibbs energy by

$$g^M = g^E + RT \sum_{i=1}^{N=3} x_i \ln x_i \quad (12)$$

The derivatives needed for Eq. (6) require that the dependent mole fraction x_N not be held constant. This can be done analytically with greater facility using the following identity:

$$\left(\frac{\partial^2 E}{\partial x_j \partial x_k} \right)_{T, P, x_N} = \left(\frac{\partial^2 E}{\partial x_j \partial x_k} \right)_{T, P, x_N} + \left(\frac{\partial^2 E}{\partial x_N^2} \right)_{T, P, x_N} - \left(\frac{\partial^2 E}{\partial x_j \partial x_N} \right)_{T, P, x_N}$$

$\frac{\partial^2 E}{\partial x_j \partial x_k}, k, N$
 $\frac{\partial^2 E}{\partial x_j \partial x_k}$
 $\frac{\partial^2 E}{\partial x_N^2}$
 $\frac{\partial^2 E}{\partial x_j \partial x_N}$

$$-\left(\frac{\partial^2 E}{\partial x_k \partial x_N}\right)_{T, P, x_l, l \neq k, N} \quad (13)$$

The second derivative of the NRTL equation for any of the terms on the right-hand side in Eq. (13) is

$$\left(\frac{\partial^2 E}{\partial x_L \partial x_M}\right)_{T, P, x_j, j \neq L, M} = \frac{G_{ML}}{B_L} \left(\tau_{ML} - \frac{A_L}{B_L}\right) + \frac{G_{LM}}{B_M} \left(\tau_{LM} - \frac{A_M}{B_M}\right) + \sum_{i=1}^{N=3} \frac{x_i G_{Mi} G_{Li}}{B_i^2} \left(\frac{2A_i}{B_i} - \tau_{Mi} - \tau_{Li}\right) \quad (14)$$

where

$$A_i = \sum_{j=1}^{N=3} x_j G_{ji} \tau_{ji} \quad , \quad \text{and}$$

$$B_i = \sum_{j=1}^{N=3} x_j G_{ji}$$

The regions identified by the combined three tests as heterogeneous are presented in Figs. E-2 and E-3 for the systems n-heptane-cyclohexane-furfural and water-xylene-pyridine. The NRTL constants for these systems are listed in Table E-1. All compositions enclosed within the curve are predicted as immiscible. These results are compared with the calculated binodal curve (Renon, 1971). As mentioned earlier, these three tests do not cover the entire region of heterogeneity, but they do provide a quick test which is worthy of consideration before more complicated methods of

Fig. E-2. Ternary diagram.

Fig. E-3. Ternary diagram.

finding tie lines are attempted. The derivative calculations for the NRTL equation as a computer program are listed below. The listings for the tests are the same as used in the synthesizer and appear in Appendix B.

Notation

a_i	activity of component i
c	matrix element
g	molar Gibbs energy
G	Gibbs energy
g^E	molar excess Gibbs energy
g^m	molar Gibbs energy of mixing
p	transformed matrix element
P	number of phases
N	number of components in system
n	number of moles
x	mole fraction
Δx	change in mole fraction
q	normalized amount of phase
τ_{ij}, G_{ij}	parameters of the NRTL equation
g	amount of pure component phase
R	gas constant

Table E-1

Parameters for NRTL examples (Renon, 1971)

(1) xylene		(2) pyridine	(3) water	
i	j	τ_{ij}	τ_{ji}	α_{ij}
1	2	-63.	282.	0.3
1	3	1934.	4314.	0.18
2	3	-90.	1615.	0.59
(1) n-heptane		(2) cyclohexane	(3) furfural	
1	2	-535.	611.	0.3
1	3	1401.	1418.	0.35
2	3	1443.	992.	0.35

where

$$G_{ji} = \exp(-\alpha_{ji} \tau_{ji})$$

APPENDIX F

Thermodynamic Routines

All of the thermodynamic routines are based on calculations using the theory of corresponding states. This allows for the estimation of many properties with very little input information needed. The input information that is needed for each component is as follows:

1. molecular weight
2. normal boiling point
3. critical temperature
4. critical pressure
5. an integer characterizing the compound as to structural homomorph.

The calculated activity coefficients which are used in almost all of the routines use a modified form of the regular solution theory (Holpinotill and Van Winkle, 1968). The two solubility parameters used in this correlation are calculated from the latent heat and the homomorph plots of varying molecular structure of Weimer and Prausnitz (1965). These homomorph plots are transformed into equations and appear in the routine SOLPAR. The latent heat and the vapor pressure are calculated from the correlation of Miller in routine VP (Miller, 1965). The compressibility factor is from Huggenmacher (1946). The critical compressibility factor and density are from Halm and Stiel (1970). SETCRIT calculates the critical properties that are not input information. SEPPAC calculates the distribution coefficients of all components based on the feed composition, atmospheric pressure, and the temperature of 130°F. Limiting activity coefficients at high dilution are used in the solvent phase for extraction, while a mole fraction of 0.637 for the solvent is used in extractive distillation.

ACKNOWLEDGMENTS

I wish to express my appreciation to Professor C. Judson King for his years of guidance in the work discussed in this thesis, and beyond.

I thank my labmates, especially Romesh Kumar and Ian Davenport, for their companionship, understanding, and contributions to my emotional well-being.

I also wish to thank Professor John M. Prausnitz for his aid in developing some of the thermodynamic routines.

This work was done under the auspices of the U. S. Atomic Energy Commission.

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