Systematic Synthesis of Separation Schemes

The paper reports efforts to automate the synthesis of separation processes. Heuristic and algorithmic programming are used to select both the sequence and types of processes used for the conversion of complex mixtures into specified products. Improved schemes are evolved using learning techniques. An illustrative example is included.

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SCOPE

Very little past work exists on the development of systematic methods for process synthesis. In an effort to understand better the underlying principles of process creation, the computer was used to build and evaluate a logical system for the synthesis of the separation train of a chemical process. The decisions incorporated into the programming are on algorithmic and heuristic (rule-of-thumb) levels. Beyond input of the initial feed conditions, a few physical properties (such as critical pressure, critical temperature, molecular weight, and normal boiling point), types of separators to be considered, and specifications on the final products, the entire synthesis is done by computer-implemented logic. Key components, types of separator, order of separation, and mass separating agent to be used are chosen in a systematic manner beginning with the initial feed. Recycle of a mass separating agent is handled where needed. The entire synthesis is repeated several times with better estimates of costs of the units, based upon results of previous process syntheses. Several process flowsheets are presented to the design engineer for his consideration.

An illustrative example is discussed in which the candidate separation processes include distillation, extractive distillation, liquid-liquid extraction, stripping, and absorption.

CONCLUSIONS AND SIGNIFICANCE

The ability of the computer to synthesize new separation schemes has been demonstrated. Several new concepts were generated as a result of the evolving programming study. 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. The cheapest-first heuristic then applies to the possible separators which could be used next while still leading ultimately to feasible sequences. The procedure of using the cheapest separator next is a generalization of several more specific heuristics.

The hierarchical ordering of executive routines in a synthesis system allows great flexibility in adding or modifying detailed simulation routines for separator units.

Process design can be roughly subdivided into two steps—synthesis and analysis. A great deal of attention has been devoted to the mathematical analysis of chemical processing systems, once the system has been specified. However, the creation, or synthesis, of that system is not very susceptible to the usual mathematical techniques and has consequently received very little attention in chemical engineering research. Process synthesis is regarded, for the most part, as an intuitive art. The purpose of this research is to make contributions toward logical structuring of process synthesis and to discover effective synthesis heuristics for use by the design engineer. The specific concern of this work is the selection and sequencing of the separation train of a chemical processing plant.

There are many possible ways of separating a multicomponent feed stream into products of chemical components, which are specified individually or as groups. Often, when the development of such a separation train is required, the design engineer will use a flowsheet scheme which has previously proven successful. He will do additional analysis, such as optimizing flow rates, temperature, and other continuous variables, but the synthesis of the flowsheet is not and at present cannot be approached in such a rigorous manner. Discrete variables must be considered, for example, either a separation unit is in the process or it is not. As an indication of the number of different sequences of units which are possible and may merit attention, consider the example of sequencing of single-feed, two-product separators which are all the same type of separation process. For simplicity, this process is chosen to be one which does not require a mass separating agent. Then the number of possible sequences for separating N components from each other into single-component products is given by the following closed-form equation:

$$\text{Number of Sequences} = \frac{[2(N-1)]!}{N!\,(N-1)!} \qquad (1)$$

For seven components the number of different sequences possible is 132. If now, instead of one type, S different types of separation process are to be considered for each constituent step in the sequence, the above formula must be multiplied by the factor S^{N-1}. With ten different types of separation process available, the 132 becomes 132 billion. It is understandably infeasible to examine individually all of the possibilities, even with a computer.

Previous studies have been reported on the sequencing of distillation units (Lockhart, 1947; Harbert, 1957; Rod and Marek, 1959; Heaven 1970; Nishimura and Hiraizumi, 1971; King, 1971). Rough, qualitative work has been done on criteria for choosing between different types of separation process for a single separation task (Souders, 1964; King, 1971). Contemporary with this work is that of Hendry and Hughes (1972), which approaches the problem of synthesizing a separation train through dynamic programming. Comparison of their approach with that used here is given by Thompson and King (1972).

GENERAL STRATEGY

It is not contended that this work is the definitive approach to the problem of flowsheet synthesis for a separation train; it is the examination of one basic approach and some variations upon it. This method does succeed in creating good schemes, without exhaustive search or large consumption of computer time. It is a venture into untrodden territory.

The purpose of this paper is to present the essential features of the approach and to summarize the experience which has been gained with it. Details of program logic and other aspects of the work are given elsewhere (Thompson and King, 1972).

The computer provides a vehicle for full documentation and subsequent assessment of the logic used in systematizing the process synthesis. The state of the 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.

The basic approach which has been implemented involves evaluating and making decisions using as little information as possible and being as general as possible. The programming has been done exclusively in FORTRAN for each of understanding by other workers, for compatibility between machines, and for more efficient coding of arithmetic operations (compared to list-processing languages). The programming done in this work incorporates several levels of executive routines, each of which, in ascending hierarchy, has less and less information available to it about the particulars of the separation units, or even about what specific chemical species are present. The routines have available to them only the information that is essential to their function. The original problem is transformed for the higher executives into Boolean-type matrices for ease of understanding and decision making, smaller core requirements, and improved speed of calculation.

At every level decisions are made heuristically as well as algorithmically. Here, an algorithm is restricted to being a mathematical procedure that necessarily reaches the desired goal; whereas a heuristic is an empirical, rule-of-thumb procedure which hopefully has a high probability of leading to the goal but cannot be shown to do so necessarily. Heuristic procedures are called for because of the complex nature of the sequencing problem and the immense number of conceivable alternative sequences.

The logic which has been evaluated and employed can best be described by explaining the interactions and workings of the various routines, along with the assumptions that went into their construction. In some cases the division of work between subroutines is rather arbitrary. The routines of most importance are defined here in overview and will later be described in detail (See Figure 1).

Although a separation unit separates components, a separation train, seen as a whole, creates products. Some or all of the products may be groups of components, rather than individual components. With this in mind, routine PROD identifies a feasible set of products for the plant. Input information includes what the designer would like as products, but these may not be possible to create without product splitting, given the available separation units. For example, components A and C may be desired in the same product, which should not contain B. However, it may be that no separation process is capable of putting B into one product stream while leaving both A and C in the other. PROD will create the desired set of products if possible; if it is not, PROD will create those specified products which are possible, and then create as few extra products as it can using the available component orderings for different types of separation processes. These extra products must ultimately be mixed in order to obtain the designer's desired products. Here a first heuristic has already been employed, namely that the best process will have the least number of products. This will not always be true, and the application of this heuristic at this point may subsequently be negated by evolu-

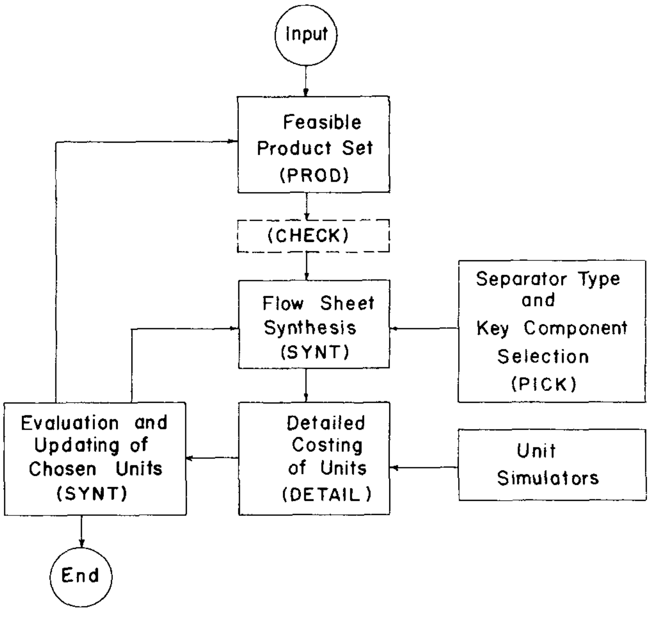

Fig. 1. General strategy.

tionary-like changes in the process configuration.

Once products have been established, a process-flowsheet which will give these products is synthesized by routine SYNT. SYNT shares some of the work with PICK, a routine which selects the next separator in the train on the basis of a second level of one or more heuristics. A heuristic which has been proven successful is that the next separation to be made is the one which can apparently be made most cheaply. SYNT handles the bookkeeping of which products are present in each stream but knows nothing about the particular chemical components which are present, except for knowing which keys are in each unit. 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 its predicted costs of different types of separators, and thus in the re-evaluation of the units in the flowsheet. 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 separation agents, is tested. Separation units on the flowsheet which are not energy-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 used. SYNT then reworks the flowsheet in the manner described above.

DESCRIPTION OF EXECUTIVE ROUTINES

For an understanding of the description of the routines it is necessary to define some of the terms used. Key components for a separation are the two components on whose split fractions the separator is designed. In this work the key components are taken as the two components to separate, that is, the pair of components, one of which appears predominately in each product, which have a separation factor closest to unity. Key products are the two ultimate products containing the key components. The light key is the key component having the greater distribution coefficient; the other is the heavy key. The distribution coefficient is arbitrarily based on the ratio of component mole fraction in the lighter state to that in the heavier state of aggregation, or, if that does not apply, in solvent phase to feed phase. These distribution coefficients are estimated by subroutine SEPFAC, which can use regular solution theory and Reidel-factor vapor pressure estimates, or can use independently specified data.

Prod

Routine PROD has effectively six entry points listed and described as follows:

(0) Initial creation of feasible product sets.
(1) Elimination of a potential product set.
(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

The desired product set is constructed as follows from the problem specification. 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 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 orders 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 Compatibility Matrix is created, indexing the pairs against themselves and also against the types of separation units. This matrix is Boolean, having nonzero elements a_{ijk} whenever pair i can be separated from pair j by separator k $(a_{ijk} = a_{jik})$. The Pair Compatibility 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 are also added to the product set as potential single-component products. The product set with the greatest number of pairs, that is, 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. This decision is later altered 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 (Figure 2) conveys to all the executive routines information on the following points:

1. Feasibility of separation between any two products by any given separation unit.

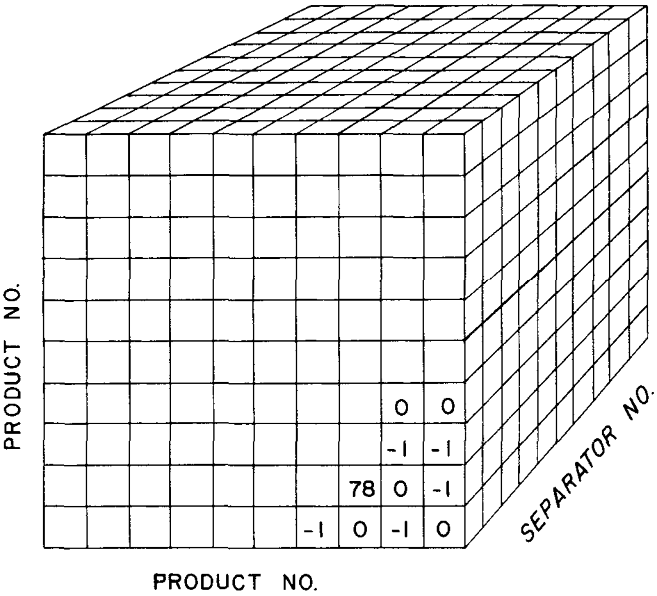

Fig. 2. Form of the product separability matrix.

2. Presence of products in the stream to be separated.

3. Separation adjacency of any two products (that is, 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.

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

Product No.	Component No.
1	7
2	8
3	5, 6

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

Separator No.	1	2	3
	5	5	5
	7	7	8
	8	6	6
	6	8	7

The Product Separability Matrix has element a_{ijk} 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 No. 1

$$\begin{array}{r|ccc} j= & 1 & 2 & 3 \\ \hline i=1 & 0 & 0 & 0 \\ 2 & -1 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

2

$$\begin{array}{r|ccc} j= & 1 & 2 & 3 \\ \hline i=1 & 0 & 0 & 0 \\ 2 & -1 & 0 & -1 \\ 3 & 0 & 0 & 0 \end{array}$$

3

$$\begin{array}{r|ccc} j= & 1 & 2 & 3 \\ \hline i=1 & 0 & -1 & -1 \\ 2 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

Any -1 entry in this matrix is a potential separation to be considered. However, for Separator No. 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.

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 the values of the nonzero entries which correspond to products that are present in the mixture (stream) and are potential key products for the separation. This alteration 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 No.

1

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

2

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 0 & 0 \\ 2 & -1 & 0 & 806 \\ 3 & 0 & 0 & 0 \end{array}$$

3

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & -1 & 706 \\ 2 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

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.

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 for the mixture of Products 2 and 3. The altered matrix now looks like this:

Separator No.

1

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

2

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & 0 & 0 \\ 2 & -1 & 0 & 806 \\ 3 & 0 & 0 & 0 \end{array}$$

3

$$\begin{array}{r|ccc} & 1 & 2 & 3 \\ \hline 1 & 0 & -1 & -1 \\ 2 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{array}$$

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 be chosen.

If PROD is called to consider another product set, a new Product Separability Matrix is created. The new product set may be one previously considered, another from the list of product sets, or a new one created by splitting a specified multicomponent product in the present set. The choice is done on command from routine SYNT. PROD is, in general, an algorithmic symbol-manipulation routine which, while making almost no judgments on its own, narrows greatly the complexity of the problem as well as the number of alternatives which need be considered.

Detailed Unit Simulation

Once the entire flowsheet has been synthesized, DETAIL is called to size and cost all of the units which are specified by SYNT. It returns to SYNT combined capital and operating costs, or information indicating that an infeasible condition for simulation has been encountered. DETAIL, in turn, calls any of the unit simulators that it needs. The routine is a sort of foreman and bookkeeper to accomplish the assigned task. All of the unit simulators require input feed components to be listed in the order of descending distribution coefficients; they also return to DETAIL lists of separator effluents ordered in like manner. DETAIL must thus reorder the components from a master list to call a simulator, and then must order back the two effluents. The master list is arbitrarily the ordering of components in the original problem statement. The routine must also add the mass separating agents to the units as required. If the feed to a specified unit is not in the required state of aggregation, a total condenser or vaporizer is inserted. Refrigeration at various levels is used where required. There are also various higher-temperature, higher-cost heating media.

The basis for sizing a unit is the specification of split fraction, specified in the original problem statement. (The possibility of a component being a key component in more than one separator and thus altering its specified recovery fraction has so far been ignored.) For extraction, absorption, and stripping, if a single-section unit fails to meet the recovery fraction specifications for both key components, DETAIL selects a second mass separating agent and calls for a simulation of a two-section column.

The unit simulators currently available to DETAIL are distillation, extractive distillation, liquid-liquid extraction, stripping, and absorption. All of them employ group methods and efficiency correlations to calculate stage requirements, flow rates, and compositions. High and low pressure operation, refrigeration, and heating media are supplied as required. Sizing and costing are based on equations fitting the data given by Peters and Timmerhaus (1968). Capital cost and yearly operating costs are weighted and combined in assigning a cost to a unit separator.

Constraints

A number of conditions can prevent completion of a simulation. These conditions are considered to be constraint violations. Some constraint violations are so severe as to warrant the elimination of that specific separator with those specific keys from ever being considered again. Two levels of violation have been established:

A. *Constraints which eliminate separation permanently*:
   1. Extreme flow ratios of internal countercurrent streams.
   2. Improper phase miscibility (or immiscibility) for the type of separator.

B. *Constraints which discourage use of separator by assigning it a high β value (see below)*:
   1. False estimation of ordering of component distribution coefficients for unit.
   2. Unit operation requires extreme temperatures.

The miscibility test involves evaluating the Gibbs energy of mixing function, along with various of its first and second derivatives for the mixture at the composition to be checked. The mixture is concluded to be heterogeneous if the derivative for any component indicates immiscibility or if there is a concave-downward shape of the free energy of mixing as a function of composition (Thompson and King, 1972). A false estimation of component ordering for a given separator results from changing distribution coefficients caused by changes in composition or temperature of the streams through the process. Such an ordering change becomes a constraint violation only if there are more than two components present and if one or more nonkey components reverse positions with respect to the keys from what was expected.

It has been found advantageous to eliminate potential constraint violations of Type A above before they occur in the detailed simulation, in fact before they can be considered as potential candidate separations. This high-level elimination is accomplished using an optional routine CHECK (see Figure 1), which is activated after PROD in alteration of the Product Separability Matrix. CHECK uses the same test as the detailed simulation for phase conditions and a slightly relaxed constraint on internal flow ratios. Separations violating these tests are removed from the Product Separability Matrix.

Synthesis

SYNT and its companion routine PICK are the heart of the programmed synthesis. Besides calling for product set creation by PROD and for sizing and costing by DETAIL, SYNT has the two main functions of synthesizing the process and improving its own ability to synthesize processes in the future. In synthesizing a flowsheet it starts with the feed stream to the process, inserts a separator, examines in turn each of the separator effluent streams for the need for further separation, and stops the synthesis when each of the final effluent streams contain only one of the products in the feasible product set. In choosing a separator, SYNT informs PICK which products are present in the stream and follows the advice of PICK as to which separator to use and as to which are the key products and components. All the products which are present in the feed to a unit are then parcelled out to the two effluent streams by examining the entries in the Product Separability Matrix. Mass separating agents to be used by a separator are also added to the appropriate effluent streams from that unit and ones downstream from it. This operation is repeated for each stream containing more than one product while each time altering the entries in the Product Separability Matrix as described earlier.

Improvement in the synthesis ability of SYNT is accomplished heuristically by a learning technique, generating weighting factors used by PICK for choosing separators. These weighting factors (β) are best understood from the equation in which they are used:

$$\text{Estimated cost of separator} = (\beta_{ijk})(N_{ijk}) \qquad (2)$$

where N is an estimate proportional to the number of stages required to separate product i from product j by separator k, under the split fractions specified in the problem. For separators having linked countercurrent flows (for example, distillation) N is the minimum number of stages at total reflux, and for mass-separating-agent processes N is the actual number of stages from the Kremser equation, with estimated absorption or stripping factors. The β weighting factors are updated after each detailed simulation of a given separator with given keys, based on the results of the costing by DETAIL:

$$\beta_{ijk} = \frac{\text{actual cost of unit}}{N_{ijk}} \qquad (3)$$

where the actual cost of the unit includes the cost of recovering the mass separating agent by a later unit, the cost of changing feed-stream state of aggregation, and/or the cost of pumping to higher pressure for successor units, if any. This actual cost may not be that at all if DETAIL finds that the use of that unit caused a constraint violation of Type B above, in which case β is given a high value to discourage further use of that separator for those keys. Initially the values of all β_{ijk} are set at the arbitrarily low value of 1 (one dollar). This encourages testing of various types of units. β_{ijk} values are often updated by groups instead of singly. For a given separator k, if one β_{ijk} has been calculated by the above procedure, then all of the other β_{ijk} for that value of k, regardless of keys, are updated to a high fraction of this value if values for that k have never been updated before. This helps the synthesizer to reject whole categories of unlikely separators.

For every stream containing more than one product, a separator must be employed. On some heuristic basis two decisions are made: (1) Which are the key products? (2) Which separator is to be used? Both of these decisions are made by routine PICK. The entire program is designed so that the majority of the heuristics to be tested can be concentrated in this subroutine. One can, for instance, split off the most volatile product, make about a 50/50 split on the products, choose least-tight splits, or whatever (King, 1971). An effective procedure has been to choose the cheapest of all separators that are candidates for being the next unit in process. In addition, some candidate separators are temporarily eliminated from contention on the basis that the separation factor between the key components is not large enough relative to distillation to make their consideration worthwhile. Extractive distillation and extraction are required to provide separation factors exceeding that for distillation by specified amounts in order to be considered as candidates (Souders, 1964).

OLEFIN-PARAFFIN SEPARATION—AN EXAMPLE

Consider the following example of a feed stream containing six components from which it is desired to make four relatively pure products. The feed rate is set at 1000 lb moles/hour.

COMPOUND	SPLIT FRACTION	DESIRED PRODUCTS				FEED MOLE FRACTION
		1	2	3	2	
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

The split fraction of each potential mass separating agent is set at 0.995. Input information also includes molecular weight, normal boiling point, critical temperature, and critical pressure. From these properties, regular-solution theory and Reidel-factor vapor pressure estimates are used by SEPFAC to generate distribution coefficients and separation factors, as called for by DETAIL and the various higher routines in the logic. Details of these procedures are given elsewhere (Thompson and King, 1972).

The following separators are to be considered for this process:

NUMBER	SEPARATOR
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; for example, 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.

PROD is called to create a feasible product set, and finds that the desired products can be produced.

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

The component numbering is given by Table 1.

TABLE 1. THE COMPONENT NUMBERING

Compound	Number
ETHANE	1
PROPANE	2
BUTANE	3
PENTANE	4
PROPENE	5
1-BUTENE	6
PHENOL	7
TETRAHYDROFURAN	8
HEXENE	9
BENZENE	10
HEPTANE	11
ISOPROPANOL	12
NITROGEN	13
EICOSANE	14
HEXAMETHYLBENZENE	15

An example of the Product Separability Matrix (for Distillation, Separator No. 1) is on the next page.

For this product set and with the routine CHECK not being employed, SYNT synthesized 15 processes that were rejected during detailed simulation due to constraint violations of miscibility and flow ratios. For example, extractive distillation when 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

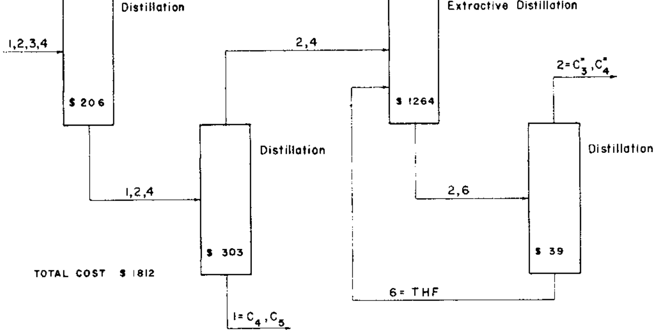

Fig. 3. Final synthesized process for Product Set No. 1—Minimum number of products ($ in thousands).

PRODUCT SEPARABILITY MATRIX

PRODUCT NO.

PRODUCT NO.	1	2	3	4	5	6	7	8	9	10	11	12	13
1	0	−1	−1	−1	0	0	0	0	0	0	−1	0	0
2	0	0	−1	0	0	0	0	0	0	0	−1	0	0
3	0	0	0	0	0	0	0	0	0	0	−1	0	0
4	0	0	−1	0	0	0	0	0	0	0	−1	0	0
5	−1	−1	−1	−1	0	−1	−1	−1	−1	−1	−1	0	0
6	−1	−1	−1	−1	0	0	0	0	0	−1	−1	0	0
7	−1	−1	−1	−1	0	−1	0	−1	0	−1	−1	0	0
8	−1	−1	−1	−1	0	−1	0	0	0	−1	−1	0	0
9	−1	−1	−1	−1	0	−1	−1	−1	0	−1	−1	0	0
10	−1	−1	−1	−1	0	0	0	0	0	0	−1	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0
12	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
13	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0	0

distillation. Solvent extractions with heptane and benzene were eliminated on the basis of solvent miscibility with the feed. Finally, an acceptable process was found (Figure 3). Furthermore, SYNT found no way of improving upon this feasible process with the given product set.

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. CHECK eliminated all 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, focusing 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 16 rejected processes (again because of constraint violation) followed by two feasible processes (see Figures 4 and 5), 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. 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.

Additional examples for other separation problems involving hydrocarbons and rare earth solutions are available (Thompson and King, 1972).

DISCUSSION

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.

Consider first the heuristic in PROD which favors the creation of product sets which make the fewest 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 crea-

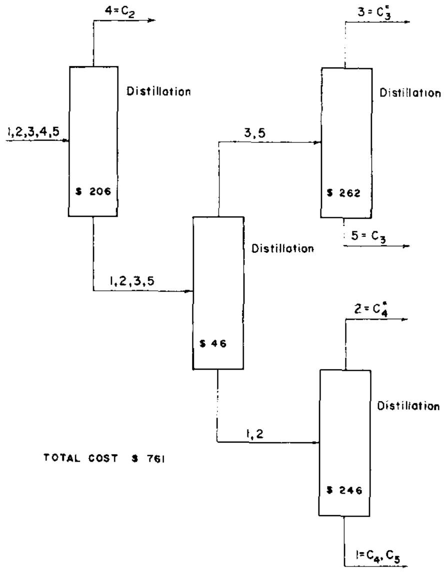

Fig. 4. Feasible synthesized process from Product Set No. 2—More than minimum number of products (\$ in thousands).

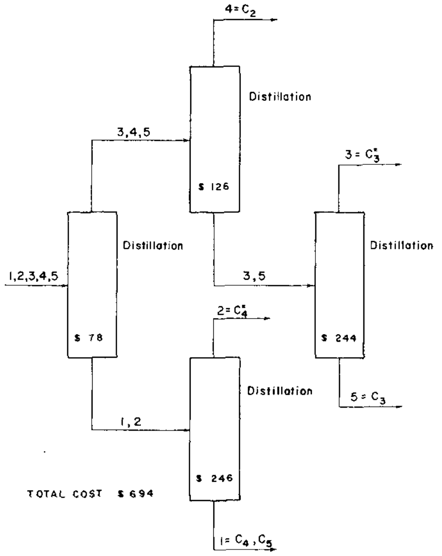

Fig. 5. Final synthesized process for Product Set No. 2—More than minimum number of products (\$ in thousands).

tion 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. In two ways separators with mass separating agents are penalized. The first is through the normal change in the β weighting factor associated with that separation. Although the product set is fixed, β reflects 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 actual cost of its implementation. This method of cost evaluation has often (in the examples run) rejected such types of separators in favor of distillation, except where a particular separation cannot be done by distillation. Often separators using mass separating agents are rejected because they violate a constraint (usually extreme flow ratios). 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 distillation alternatives 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 example cited above, the implementation of this heuristic procedure resulted in a lower cost process.

Process improvement through the updating of weighting factors, although usually successful, has failed on occasion by cycling between two processes, each using the same separators and key products but in different sequential ordering. The β values reflect the type of separator and the keys used but not the position in the process. The presence of nonkey components in the units can radically affect the cost (consider 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. A good solution here is yet to be found.

The heuristic of beginning at the feed to the process and inserting the cheapest available of the feasible candidate separators for the given product set (cheapest first) has most often been successful. It has failed when the synthesizer cycles between processes, when flows build up in size toward the end of a separation train (such as for repeated separation of dilute solutions by means of solvent extraction), and in other cases where the cost of a unit is strongly dependent upon its position in the process (see Thompson and King, 1972). Its implementation uses very little computation time and it accomplishes what many other more specific sequencing heuristics seek to do (King, 1971). Leaving the most difficult separations, both in terms of separation factor and in terms of split fraction, until all nonkeys have been removed is a natural consequence of cheapest first. Having subsequent units at lower pressure is also a result of this heuristic since the upstream unit is charged for the cost of raising the pressure of its effluents to meet the requirements of successor units. No heuristic used yet has favored a 50/50 split of flows through the separators, although it is known there should be some incentive for this (Harbert, 1957).

A chief thrust of this work has been the reduction of problem size, or search space, by the identification of infeasible solutions as early in the computation as possible. PROD does a very good job here. It provides a product set that is guaranteed to be feasibly produced, and it allows consideration of only the feasible separators throughout the synthesis procedure through the alteration of the Product Separability Matrix. Earlier identification of infeasible conditions arising in the detailed simulation of the units, so that such units are not chosen in the first place, is performed well by CHECK, as seen in the example problem.

The approach to the problem of process synthesis that is taken here requires almost no simplifying assumptions. Separation factors can change radically with changing composition of the various streams. Such changes are handled well. There is no requirement that mass separating agents must be recovered immediately following their use. Products may be single or multicomponent. Detailed simulation of the units may be made as complex as desired. The work presented here is not intended as a specific computer program for immediate use in creating separation trains but as a vehicle for the development and understanding of concepts of process synthesis.

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