APPLICATIONS OF SYSTEMS SYNTHESIS TECHNIQUES TO INDUSTRIAL SYSTEMS

by

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B. S., Kansas State University, 1973

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1975

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ACKNOWLEDGMENTS

My Master's thesis would not have been possible without the assistance of the following people. Dr. P. N. Mishra introduced me to systems synthesis. Herbert Chen developed in me a practical understanding of chemical engineering and supplied the optimization routine used in my example problems. Dr. L. T. Fan taught me the importance of completeness. My parents supported me with their faith. Rosemary, my wife, and Katie, my daughter, gave me, with their love, patience, and unselfishness, the dedication to continue.

Financial support for this work was supplied by the Kansas State Engineering Experiment Station.

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CHAPTER 1

INTRODUCTION

Systems synthesis is the optimization of a process with respect to not only the independent variables associated with the various units in the process, but also with respect to the structure, the interconnections between units and the existence of units.

This thesis will explore the present methods, and applications of system synthesis in order to judge the applicability of each method to large industrial problems. A review is performed to briefly trace the development of systems synthesis, but more importantly, to review the most recent methods and applications of systems synthesis. The emphasis is toward finding a technique that can solve large, complex industrial design problems. Applications of the methods of systems synthesis are applied to two example problems.

Each problem is solved completely with the method which appears to be applicable to that particular problem. In addition, all of the other techniques that have been used in systems synthesis are discussed with respect to the particular problem.

The state of the art of systems synthesis is finally evaluated and a direction of future research is defined.

CHAPTER 2

A REVIEW OF SYSTEMS SYNTHESIS

The study of system synthesis, beginning in 1968, has developed into six major areas; the decomposition approach, the heuristic technique, evolutionary design, dynamic programming, branch and bound strategies, and the structural parameter integrated approach. How one classifies a particular application can be somewhat subjective since many papers use combinations of these basic techniques. To describe system synthesis, the guides for type assignment must be somewhat soft or flexible so that a single paper can be said to advance more than one concept of synthesis.

Two earlier studies by Hendry and Rudd (1973) and Osakada and Fan (1972) were excellent works on the beginnings of this discipline. Each reviewed virtually every paper on systems synthesis before 1973. This review will not attempt to cover in detail the beginning of systems synthesis, but will emphasize the progress since 1972. Of course, to review an area of study without noting the beginnings would also be misguided but, again, the emphasis will be on the later developments.

METHODS OF SYSTEMS SYNTHESIS

Decomposition Approaches

To decompose is to subdivide; to subdivide is to simplify. Rudd (1968) first formally stated the decomposition algorithm for the optimal design of a complicated or nonsolvable system as one of decomposing the original problem into smaller solvable problems. For the simplest case, one large system is decomposed into two smaller subsystems, or one large optimization, design problem is decomposed into two smaller less complicated, solvable optimization problems and one problem of optimally recombining the subsystems into the large, original system. The subsystems are optimized with respect to the independent variables associated with each subsystem, and the decomposition, recombination problem is optimized with respect to how the problem is decomposed and recombined.

Rudd describes a general philosophy of developing a design as one of decomposing a problem that cannot be solved with existing technology into a group of subproblems which can be solved with existing technology.

Several researchers have investigated how large sets of interconnected equations can be solved by decomposing the problem into smaller tasks and then combining the smaller problems into the original large problem.

Christenson (1967) investigated the problem of decomposition of design equations for large systems with many recycle streams in order to produce a solution procedure and an optimal solution.

One of the most recent of these solution procedures, tearing algorithm papers, was that by Westerberg and Debrosse (1973). Again it presents a method to obtain a solution procedure for a system with many recycle streams and other complicated interconnections.

Decomposition procedures have been applied to the systems synthesis problem directly by Nishida et al. (1971), Kobayashi et al. (1971), Umeda and Ichikawa (1972), Menzies and Johnson (1972) and Osakada and Fan (1972).

In 1972, a symposium was held in Cambridge, England, on decomposition theory as applied to control theory, computer science, operations research, chemical engineering mathematics, and network theory. The notes of the symposium, edited by Himmelblau (1973), contained thirty-seven papers. About ten papers considered nonlinear systems, but only two of these papers presented complete applications of their proposed decomposition schemes. The first paper by Westerberg implied that the direct solution of a combined problem without decomposition could be obtained more quickly than the decomposed problem. Jung (1973) also reported this result when he reviewed several decomposition schemes. The second paper from the symposium by Sandbloom illustrated the optimization of a highly decomposable system of equations with his proposed decomposition scheme. The results indicated that, again, the direct solution without decomposition was faster than the decomposed problem. The method also required that the objective function and constraints were convex and differentiable functions. Of course, the equations normally encountered in systems synthesis studies may not be convex or differentiable.

Wilde (1972) computed the constrained derivative from each stage of a large interconnected system and then the entire system is constructed from the combination of the derivatives of each stage by the chain rule.

Umeda (1972) has presented the concept of a feasible decomposition method. All decomposition procedures before Umeda's decomposed a problem by assigning a variable at one point in the procedure and at some later point in the solution procedure, an equality constraint was added. The effect is to require the production of infeasible regions. Umeda's method first requires that the number of coordination variables produced in a decomposition is less than the number of independent variables associated with all of the subproblem optimizations. Next, instead of relaxing an equality, Umeda used one of the internal independent variables in the subsystem to fix a coordination variable. An iterative technique is then used to alternatively fix coordination variables by selecting internal independent variables associated with a subproblem and, secondly, by selecting the remaining independent variables to achieve the desired result in the objective function.

Umeda's technique of feasible decomposition is the first method that considers the relative number of coordination variables and internal independent variables. Many times, a problem has been considered complicated with nine independent variables so that it is decomposed to a set of problems. Two of the subproblems contain four independent variables, one problem contains one variable, and the coordination problem of recombining the system contains thirteen variables. Such strategies are doomed to fail in general applications.

Umeda's procedure is also limited in that it must be possible to invent a solution procedure so that a coordination variable can be fixed by fixing an independent variable associated with a sub-unit. This, in general, cannot be accomplished.

Heuristic Technique

A heuristic rule is a guideline. Usually, its validity has been found from experience as opposed to being proved exactly. In engineering the existence of such rules is wide spread. Indeed, the most noticeable distinction between a practicing engineer and a new graduate entering the field is the heuristic-knowledge gap.

Before the increased studies in systems synthesis, only heuristic rules were available to assist the design engineer. Probably heuristic rules are still used more often than any system synthesis technique yet developed.

The systematic use of a set of heuristic rules and a learning technique in systems synthesis was first attempted by Masso and Rudd (1969) in heat exchanger network design.

Guidelines in design on heuristics are used in every industrial simulation, optimization, or systems synthesis study, but when the decisions regarding the existence of, the order of, or the operation of the processing units is determined by the selection of a heuristic rule from a set of equally applicable, but not equally selectable, heuristic rules then the systems synthesis technique will be called a "heuristic technique." The technique is applied by first developing several sets of possible heuristic rules. The selection of which heuristic rule should be used is then determined by additional sets of weighting terms. An iterative process is used. Every time a particular heuristic rule performs well, its respective weighting term is incremented; if the heuristic rule performs poorly, the weighting term is decremented. The value of the weighting term then determines which heuristic rule will be used from that set during later iterations.

Thompson and King (1972) used the heuristic technique to generate separation sequencing solutions. The heuristic rules used in this study were developed by Heaven (1969) in his study on distillation sequencing.

Siirola and Rudd (1971) extended the heuristic technique so that, given a reaction sequence, a complete task identification procedure could be developed, including material and energy balances and utility estimates. In addition to the heuristic rules employed in the computer program, the provision for the interaction with the design engineer is also included. Siirola, Powers, and Rudd (1971) continued with this Adaptive Initial Design Synthesizer (AIDES) and developed a semi-automated design synthesizer. This final form performs the complete design problem from the reaction scheme to the final flow sheet with the complete equipment specification.

Since the work of Powers in 1972, no new techniques or papers have been proposed dealing with the heuristic technique.

Evolutionary Method

A basic design technique used by practicing engineers in industry is evolutionary design. The principle is to first start with a working system and improve it. Of course, how or where the improvements should be made is not obvious. Indeed, that is the challenge to industrial optimization, to find areas in a system where costs can be decreased.

This method of evolutionary design is also used in systems synthesis. Again, the starting point is a working, feasible design. From this point changes are made in the structure of the system and the effect on the objective function of the proposed system is observed. If the profit is increased by the change in structure, the new system replaces the original design.

Evolutionary design has been used by King, Gantz, and Barnes (1972) to reduce the ethylene loss from a demethanizing tower of a chemical complex. How and where the changes in structure were made was determined entirely by engineering judgement. In effect, the system was studied to such an extent that possible changes were uncovered.

In the next problem, a set of rules were employed to find where a change should be made in the design. In this case, an available energy balance was performed over the entire process. Those units that had the largest loss of available energy were then studied more closely in order to determine some possible structural change. This new method was employed by King et al. (1972) to minimize the energy used per pound of liquified methane produced in a liquification process.

Ichikawa and Fan (1972) used the evolutionary process to design a reaction, separation system. In addition, they derived the necessary condition for an optimal system, yet the individual changes in structure were obtained by engineering judgement.

The dual feasible decomposition proposed by Lasdon (1970) was used by McGalliard and Westerberg (1972) to develop an evolutionary design procedure with which the effect of a structural change could be determined without reoptimization of the entire system. Several heat exchanger network designs were synthesized with satisfactory results.

Dynamic Programming

A waste treatment plant was synthesized using dynamic programming by Shih and Krishnan (1973). The paper does not consider the problem as one of systems synthesis but, since the systems approach used considers the existence of various streams and units, the problem is really one of systems synthesis. The system concerned has a primary clarifier, a trickling filter, an aerated lagoon, an activated sludge reactor, coagulation sedimentation, and filtration with carbon adsorbent. A major drawback in the problem formulation was the lack of a recycle stream around the activated sludge reactor. In practice, such systems are extremely rare.

Separation sequencing was first performed with dynamic programming and list processing by Hendry (1972). The difference between a pure dynamic programming solution to the problem and the inclusion of list processing was two-fold. First, the number of possible sequences that had to be considered were reduced by only allowing those separations included in the list processing scheme. In other words, only a single split could be obtained for each separation. The second difference was that the list processing scheme allowed all types of separations to be considered in the same dynamic programming problem. Extraction, distillation, crystallization could all be considered in the same separation sequencing problem.

Energy integration was added to the work of Hendry by Rathore (1974a,b). By using Hendry's method of separation sequencing and dynamic programming for the heat exchanger network design, the integration was achieved. In a second paper, the problem was extended to the sequencing problem with distillation towers with pressures other than atmospheric. Branch and bound was used for the heat exchanger network design in this second paper. Optimal systems were obtained by both techniques but the relative savings was small over systems without energy integration.

Branch and Bound

Only three applications of branch and bound have been formulated in the study of systems synthesis. Heat exchanger network synthesis was performed by Lee and Masso (1970) by using a branch and bound algorithm. By relaxing the network feasibility criteria of only using a stream once in a network, a branch and bound algorithm could be formulated. A cost matrix was completely constructed from the costs of individual exchangers and subsequent networks including the necessary utility steam and cold water needed to accomplish the process. The step of filling the cost matrix was considered to be the simplest step in the design problem. Next various branching strategies were developed along with the appropriate bounding criteria. By the repeatedly branching and bounding, the original problem was transformed into many small problems, many of which would not have to be solved completely. The job of comparison was then drastically reduced.

The second application of branch and bound by Menzies and Johnson (1972) expanded Lee's basic method of heat exchanger network design by considering both the heat transfer problem and the pressure change problem. The systems structure for the units other than the heat exchanger network was fixed for the entire problem.

Branch and bound was finally used by Rathore (1974b) in his distillation sequencing and energy integration problem.

Feasible Matrix and Decision Tree Methods

A decision tree algorithm developed by Pho and Lapidus (1973) has been proposed that considers only the feasible structures of heat exchanger network synthesis. By judiciously assigning stream matches in a matrix representation the assignment problem can be reduced and the computational burden is directly reduced. The condition that allowed branch and bound to be used in heat exchanger network synthesis was the relaxed constraint on the multiple use of a single stream. The tree structuring method can then be used to include the multiple use constraint and therefore reduce the required computation. In other words, a four stream example stated by Lee required the evaluation of 4200 possible system structures with the refinements of branch and bound only a small number of structures had to be compared in order to obtain the optimum structure. But with the use of the decision tree structuring of stream matches, only twenty-one structures had to be examined in order to determine the respective cost, and all of the possible feasible structures exist in this list. For small problems, the entire tree can be enumerated to find the optimal structure. Refinements in the procedures allow only the partial enumeration of the tree structure in order to arrive at an optimal or near optimal solution.

Synthesis by Direct Optimization

The structural parameter of solution formulation was introduced and first used with a direct search by Ichikawa et al. (1969), and has been used extensively. Since the study of optimization has been so extensive, it would seem plausible that these techniques could be used directly in systems synthesis. This is the basis for the structural parameter method of solution formulation used with a direct search. The method begins by devising a system structure composed of all the reasonable combinations of units. Engineering judgement and basic heuristic rules must, of course, be used in order to devise both a general system and a system of moderate size. Structural parameters are employed at splitting points to determine the split fractions of the state variables to the various streams leaving the split point. After a solution procedure and the appropriate decision variables are obtained, the system can then be optimized with any existing nonlinear optimization technique.

Since structural parameters are mere splitting fractions, they may be used in combination with other systems synthesis techniques, as opposed to being only used with a direct search. Umeda and Ichikawa (1972) used structural parameters with a decomposition technique. Ichikawa and Fan (1972) used structural parameters with an evolutionary approach. Umeda, Shindo, and Tazaki (1972) used them with a feasible decomposition technique.

Hybrid Methods in Synthesis

Combinations of methods is very common in systems synthesis. Fig. 2-1 illustrates the papers that used several methods in their approach. For example, Hendry (1972) used both dynamic programming and list processing in order to accomplish his separation sequencing. Rathore et al. (1974a,b) then followed Hendry and added the branch and bound strategy devised by Lee et al. (1970) to integrate the energy and separation sequencing problems.

Ichikawa and Fan (1972) used the structural parameter method of solution formulation and an evolutionary approach to optimize a reactor separation system. Osakada and Fan (1972) used the structural parameter method of solution formulation and a decomposition multileveled procedure to optimize a reaction separation system.

THIS BOOK CONTAINS NUMEROUS PAGES WITH DIAGRAMS THAT ARE CROOKED COMPARED TO THE REST OF THE INFORMATION ON THE PAGE.

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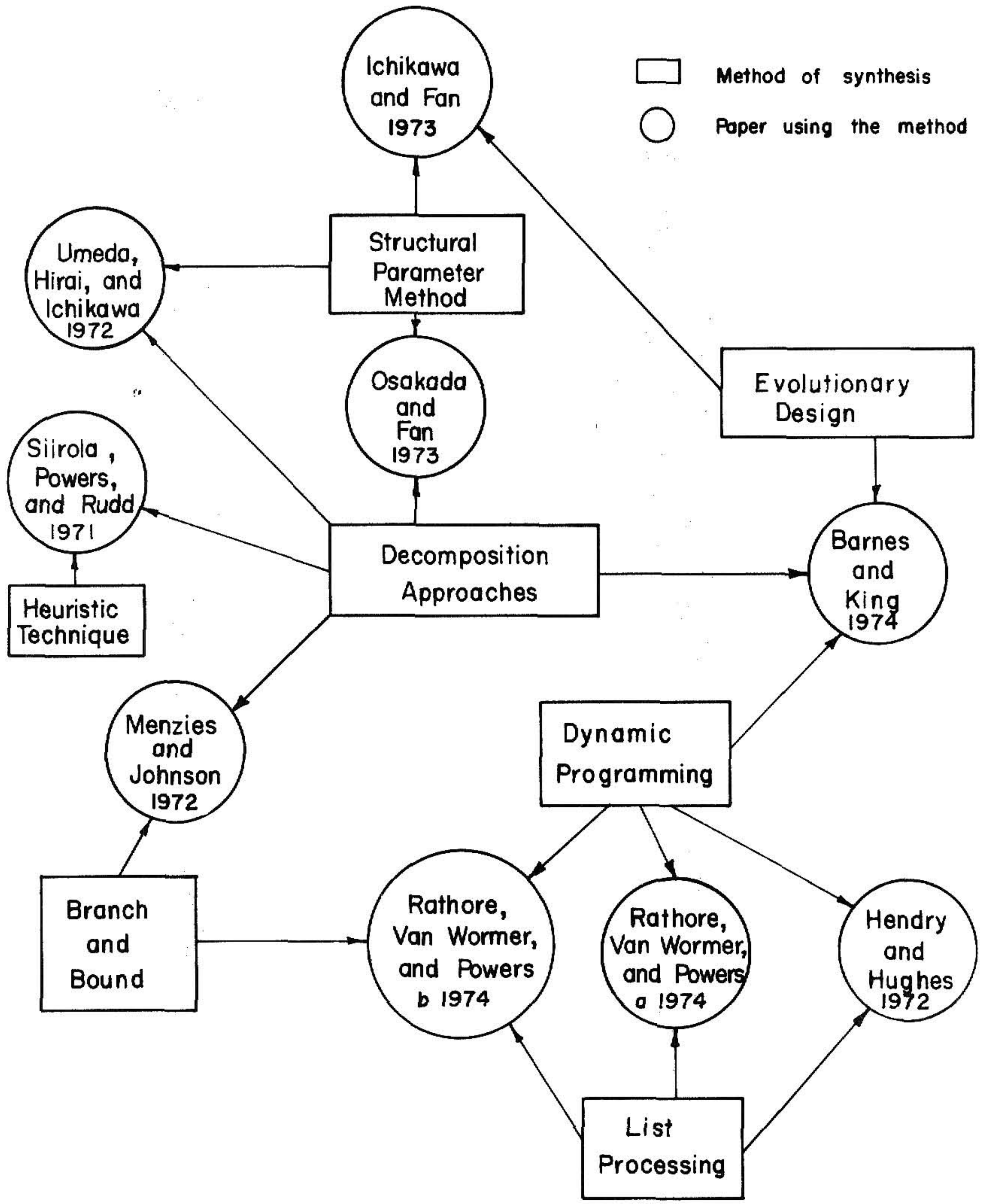


Fig. 2-1. An illustration of hybrid systems synthesis techniques.

In Fig. 2-1, only those approaches that used a combination of techniques appear. Obvious exclusions have been the works of Lee et al (1970) and Thompson and King (1972). King (1972) used both the evolutionary approach and the heuristic approach in separate papers but he didn't ever combine the two techniques.

APPLICATIONS OF SYSTEMS SYNTHESIS

Homogeneous Systems

Separation sequencing. In the design of separations sequences, there are two outstanding areas of study. The first is the "heuristic technique" proposed by Thompson and King (1972). The Rudd, Siirola, and Powers group first established the heuristic technique in systems synthesis but their application to separation sequencing has been with a heterogeneous system.

Thompson and King's (1972) approach is very similar to the approach described in the earlier section on the heuristic technique.

Hendry (1972) used dynamic programming to devise separational sequencing. He was able to reduce the size of the problem with the application of a list processing technique to trim the infeasible branches from the decision tree. For large problems, the decision tree becomes very large so that this approach is limited to smaller sequencing problems.

In summary, when a problem increases in size, as in the separation sequencing, a heuristic technique, approximate solution must be used. Exact procedures such as Hendry's method become impractical.

Reactor network design. Dynamic programming was applied to the design of reactor networks by Aris (1969). In this problem, the structure, or type of arrangement, was fixed but the number of reactors used was variable. The problem was then one in systems synthesis.

When considering non-ideal reactor systems as a plug flow system with localized mixing, Jackson (1968) developed a reactor sequence using a variational technique. The problem considered the optimal placement of a fixed volume CSTR between two portions of a fixed total volume plug flow reactor.

Several systems have been generated using structural parameters in the solution formulation. A plug flow, CSTR reactor system with a perfect separator has been synthesized by Osakada and Fan (1972) and by Ichikawa and Fan (1972). Umeda and Ichikawa (1972) synthesized a CSTR and plug flow reactor system.

The synthesis of an extractive reactor system was done by Masakaza and Matsubara (1974). This can be said to be a combination of a CSTR reactor and a separator system. The problem is a homogeneous systems synthesis problem made up of heterogeneous units. Structural parameters have been used in the solution formulation with a direct search. Several different numbers of extractive reactors were used and an optimal solution was obtained for each different system.

Heat exchanger network design. The two best techniques that have been used in the synthesis of heat exchanger networks that are not limited by linear models are branch and bound and the feasible matrix, decision tree method.

Branch and bound is a well-known technique for combinatorial and assignment problems. It was first applied to heat exchanger network synthesis by Lee and Masso (1970).

In order to apply branch and bound to the heat exchanger network design, a feasibility constraint had to temporarily drop. Many nonfeasible networks could then be established for very small problems. A four stream problem had a total of 4200 possible feasible and nonfeasible structures.

In the inception of the method, three steps had been envisioned in the synthesis of such networks: cost evaluation, cost comparison, and feasibility evaluation. At this point, the assumption was made that the most time-consuming step was the comparison step, therefore, the computation step, the cost evaluation, was assumed to be trivial. The method then concerns itself to a large part with more efficient methods of determining the optimal network with cost comparisons and by determining the network's feasibility. Siirola (1974) indicated that the branch and bound method was the best method for heat exchanger synthesis, but he had not included the feasible matrix and decision tree method in his comparison.

The feasible matrix and tree approach by Pho and Lapidus (1974) does not drop the feasibility constraint of the multiple use of a single stream. Therefore, every network considered is feasible. The reduction in the number of heat exchanger networks for which costs must be computed is drastically reduced from that required by branch and bound. A four stream problem in branch and bound needed the generation of 4200 cost evaluations, but the feasible matrix and decision tree method needs only 21 cost evaluations. For small problems of seven streams, the complete decision tree can be evaluated. For larger problems a look-ahead technique is used to help direct the partial enumeration of the decision tree.

Heterogeneous Systems

Energy exchange networks. Evolutionary design was used in energy exchange networks by King, Gantz, and Barnes (1972). They used a technique very close to the one described in the earlier section on evolutionary design.

Barnes and King (1974) designed a cascade refrigeration and liquification system by first using a graphical decomposition technique to locate a set of optimal or near optimal strategies. Each of these designs was analyzed in more detail with dynamic programming. Finally, the process is repeated iteratively to obtain the optimal solution.

A slightly different slant on the problem of energy exchange network design is given by Umeda, Shindo, and Ichikawa (1974). They assumed that the major equipment design, the reactors, separators, and mixing equipment, for the system had been fixed by either the pioneering work of a research group or perhaps the dictates of a supervisor. The resulting problem then consisted of optimally adding the heat exchangers and pressure changing units in order to connect the basic preassigned units.

The problem by Umeda, Shindo, and Ichikawa (1974) was solved with a multileveled technique. On the top level, input temperatures and pressures to the various task assignments, those sub-units needed to accomplish the heat exchange and pressure change, were assigned. Two smaller sublevels were then devised to accomplish the optimal design of the subtask units. Of course, the output temperatures of the heat exchanger subtask and the output pressures of the pressure change subtask may not match those designated in the top coordination level. An iteration is then required over the entire process. One major difference between the basic formulation of this system synthesis problem and any other is that no specific method is required in the sub-optimization of the sublevel problems of heat exchange and pressure change. In this example problem, the heat exchange subtasks were optimized by Kobayashi and Umeda's (1971) method of heat exchanger network design.

Entire process design. Few researchers have approached the problem of complete chemical plant design; in fact, only two methods have been applied to this total problem.

Siirola, Powers, and Rudd (1972) applied, first, a decomposition approach and, secondly, the heuristic technique to develop a computer program that solves the total problem of heterogeneous chemical plant design. Unfortunately, the heuristic technique used does not yet supply information about heuristics as applied to general design problems. The major advantage of the heuristic technique as applied to large problems that the heuristic rule can be adjusted so that a less exact solution can be obtained by reducing the specific nature of the heuristic rule. Problems with the heuristic technique include the arbitrary nature of both the heuristic rules used and the methods used to adjust the weighting terms that decide in a later iteration which heuristic should be used.

The structural parameter method of solution formulation is the only other basic technique that has been applied to total plant design. A CSTR reactor, a plug flow reactor, and a perfect separator design has been solved in connection with decomposition by Osakada and Fan (1973) and with a random direct search by Fan and Mishra (1974).

Umeda and Ichikawa (1972) developed a design problem considering a reactor network consisting of two CSTR reactors, a distillation system with two distillation columns, and the additional heat exchangers and pumps required for the existing streams.

In areas of biological processing, waste treatment and food production, two researchers have used structural parameters in the design of their respective systems. Fan, et al. (1973) designed a waste treatment facility with both an active sludge and a trickling filter biological processing unit. In addition, a secondary settling tank and recycle was considered in the system. The results should be more accurate than those of Shih and

Krishnan (1973) who used no recycle streams so that a straight forward dynamic programming procedure could be employed.

Heydweiller (1974) used the structural parameter solution formulation to design a multi-staged tower fermenter, in which both back flow and recycle were considered.

The major problem with the structural parameter solution formulation is the inherent increase in dimensionality associated with practical, large scale problems. In addition, the excessive engineering design knowledge may be needed to establish the original basic design.

A difference between the heuristic technique and the structural parameter solution formulation approach is when the engineering judgement decisions are made. In the structural parameter method of solution formulation the decision on the number of basic processing units and the types of processing units is made at the beginning of the problem. But in the heuristic technique, more, smaller heuristic rules are applied in order to pick the types and numbers of units and the structure of the process. The possibility of obtaining information about basic systems synthesis from the learning methods used in the heuristic technique has yet to be realized and, therefore, this advantage cannot be considered.

Reaction path synthesis. An extension to the decomposition theory used in AIDES has been the basis for the study into the optimal reaction path theory by Powers and Jones (1973). The decomposition approach in AIDES assumes that the reaction is the basis on which an entire processing scheme can be designed, but the specification of the reaction at the time of AIDES could not be made. Reaction path synthesis is an attempt to bridge the final gap between a set of raw materials and a product set with specified purity.

The method applied to reaction path synthesis by Powers and Jones (1973) has been a dynamic programming and list processing approach very similar to that applied to separation sequencing by Hendry and Hughes (1972), except that minimization of time needed is considered as the objective as opposed to the economic consideration. Some large chemical synthesis problems solved with this technique have had processing sequences very close to those found by the exhaustive searches of the applied chemists synthesizing the same component.

Theorem proving. The techniques of artificial intelligence first applied to systems synthesis by Masso and Rudd (1969) have been reinvestigated by Mahalce (1974). A theorem-proving procedure has been advanced as a possible method of systems synthesis.

Basically, the method begins by establishing a set of actions, a set of conditions, and a set of results. Conceptually the set of actions corresponds to the raw materials and their conditions of temperature, pressure, and concentration. The set of conditions correspond to the laws of thermodynamics, the practical considerations of transport phenomena, and the state of the art of design. Finally, the set of results is the desired set of products and their conditions of temperature, pressure, and concentration. A very crude example of the entire method would be the production of 100 pounds of saturated steam at a pressure of 10 atmospheres. The raw materials are taken as 100 pounds of water at 75°F. If the set of conditions of this problem were that, within the present technology, 10% of the water used in making steam is lost, then the proposed problem of making steam from 100 pounds of water would be considered infeasible. A trace-back technique could then be used to determine the condition that caused the infeasibility of the process. The amount of raw material, the action, would be changed and the process would be considered feasible.

In the paper presented by Mahalce (1974), no economic criterion was considered so that the theorem proving method as applied to optimal systems synthesis is not complete. Indeed, as the above example indicates, without economic considerations, the method can at most determine feasibility.

Another difficulty with the theorem proving algorithm is how the total accumulated knowledge of, or at least the appropriate subset of, the fields of thermodynamics, transportation, and the practical design theory can be translated into a coherent set of conditions.

Finally, the linkage between an economic cost-computer routine is assumed to be a small problem. Indeed the linkage between the theorem proving algorithm and the economic subprogram may be a small problem, but the generation of an optimal design from this theorem proving algorithm based on an economic criterion is not trivial. The route a particular solution will follow from the action set through the condition set to the result set is only controlled by the existence of a possible path. Therefore, the generation of optimal systems cannot be necessarily obtained from the theorem proving algorithm. Only the feasibility of converting the action set to the result set can be determined. How the economic problem can control the structuring problem is the study of systems synthesis.

CHAPTER 3

COOLING SYSTEMS SYNTHESIS FOR POWER PLANTS

INTRODUCTION

A cooling system is one of the basic units of the electric power generating plant. Only 40% of the energy received from the fuel (coal, gas, oil, or nuclear) is converted to usable electric power. The lost energy is in the form of heat which must be removed from the system. The cooling system is the means of removing this heat from the power plant.

A condenser is the first step in the heat removal cycle. Water is used to condense a low pressure steam from the turbine. The heated water then flows from the condenser to the next phase of the cooling system where the heat is transferred to the atmosphere. The types of units needed for this operating include cooling ponds, dry mechanical draft cooling towers, wet mechanical draft cooling towers, and natural draft cooling towers as described by Krenkel and Parker (1969) and Riegelman (1971).

The cooling pond is merely a larger reservoir through which the heated water flows. The heat in the water is then transferred to the air by mechanisms of conduction, convection, and some evaporation of the water. An advantage of cooling ponds over other units is a low operating cost, usually only a pumping cost need be considered. Disadvantages of the pond include a large initial capital investment, a large land area is needed, and large evaporation loss of the water, on the order of 5% of the total water flow rate through the pond.

A dry mechanical draft cooling tower is a large one pass air cooled heat exchanger. Its basic advantage is an almost zero evaporation loss of water. This becomes very important when the cost of water is high, due to treatment costs or if water is scarce as in arid regions. The disadvantages of a dry cooling tower include a very large capital investment and a large operating expense since both fans and pumps must be used.

The mechanical draft wet cooling tower is basically a counter current packed column with water flowing down due to gravity and air flowing up because of the mechanical draft. The advantage of this tower is that the initial expense is usually lower than the mechanical draft dry cooling tower, the pond, or the natural draft tower, but the operating expenses for the pumping and blower costs usually are high.

Natural draft towers may be wet or dry. The difference between a mechanical or natural draft is that the natural draft towers use only the relatively low density of the heated air to force the air through the tower. The advantage of these towers is a lower operation cost because no fan is needed, but the disadvantage is a high initial cost.

Design of cooling systems has usually entailed the arbitrary selection of one of the various types of units, either a pond or one type of tower and subsequent sizing. Costs are then calculated for perhaps two other types of units, but rarely has this design been approached as a problem in systems synthesis.

Two researchers have considered the design of cooling systems as a problem in systems synthesis. The first, Gupta (1973), considered the combined system of a dry mechanical draft cooling tower and a pond. In his study a high cost of water was assumed as if the system were to be used in an arid area. Also a fan operating cost was considered in the optimization. Several of the optimum systems generated by Gupta were combinations of the tower and the pond, with substantial decreases, in cost as opposed to homogeneous system costs.

Fan and Lin (1975) studied the cooling system design by using systems synthesis and more than one type of unit. They considered a cooling system where water from a nearby river was used for cooling. The water was returned to the river after it had passed through both the condenser and the tower, pond cooling system at a temperature equal to or greater than the average stream temperature. In the problem formulation by Fan and Lin (1975) only the initial capital expense of the units was considered and all of the temperatures of the system were fixed. Their results indicated that the only variable in the optimal selection of a cooling system was the cost of the land on which the pond was built. No combination of tower and pond was found to be optimal. Only systems with homogeneous elements, either a tower or a pond, were optimal.

This present study has extended the system studied by Fan and Lin (1975) by including the operating expense of the entire cooling system and by allowing various temperatures to become variables. The operating expense will include both the cost for the fan, and the pumping cost for the tower, pond, and condenser.

In Fan and Lin's (1975) work all of the temperatures of the cooling process were fixed. The optimization problem was then a linear programming problem, in which heterogeneous combinations of a cooling pond and a cooling tower could not be optimal. This present work considers two temperatures, the temperature of the cooling water leaving the tower, T_{TC}, and the temperature of the cooling water entering the power plant, T_C, as in independent variables. This optimization problem is no longer linear, so that heterogeneous combinations of the cooling tower and cooling pond can be optimal. Since the temperature is a variable, two constraints are to be included to bound the optimization problem These constraints limit the velocity of the flowing water in both the condenser and the transportation lines to be less than ten feet per second.

COST MODELS

Cooling Tower Capital Costs

The cost model used to predict the cooling tower initial capital cost is based on the fundamental design equations used in the cooling tower industry for both the mechanical draft and natural draft wet cooling tower as described by the Cooling Tower Institute (1967). A simplified derivation is presented in this paper but an exact derivation can be found in the works by Gurney (1966) or Kern (1950).

The wet cooling tower is a counter current packed column. Figure 3-1 represents the tower. An energy balance about the tower gives the following results.

$$\rho\, W\, C_{pw}\, (T_{TH} - T_{TC}) = G(h_2 - h_1)$$

or

$$\frac{\rho\, W\, C_{pw}\, (T_{TH} - T_{TC})}{G} + h_1 = h_2 \qquad (3.1)$$

Therefore equation (3.1), if plotted on an enthalpy vs. temperature graph, is a straight line. This line is called the operating line. If we assume the Merkel equation (Kern, 1950),

$$Wdt = K'a'dV'(h' - h) \qquad (3.2)$$

By letting $dV' = A'dL'$

$$dL' = \frac{W}{K'aA'} \frac{dt}{(h' - h)} \qquad (3.3)$$

Integration yields

$$L' = \frac{W}{K'aA'} \int_{T_{TC}}^{T_{TH}} \frac{dt}{(h' - h)} \qquad (3.4)$$

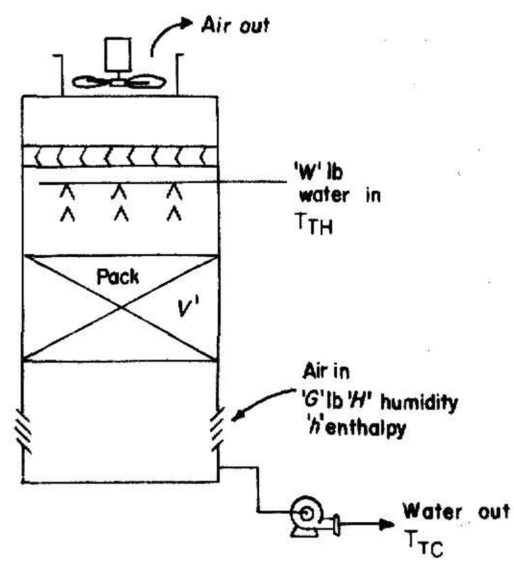


Fig. 3-1. A representation of a wet cooling tower.

where

L' = height of the tower

$\frac{W'}{K'aA}$ = height of the transfer unit, ft.

T_{TH} = temperature of water entering cooling tower

$\frac{dt}{(h' - h)}$ = number of transfer units

T_{TC} = temperature of water leaving cooling tower

W = water mass flow rate, $lbm/(hr.\ ft^2)$

a' = transfer area per unit volume, ft^2/ft^3

A' = area of the tower, ft^2

K' = mass transfer coefficient, $lbm/(hr\ ft^2)$

h = enthalpy of air, Btu/lbm

h' = enthalpy of the saturate air, Btu/lbm dry gas

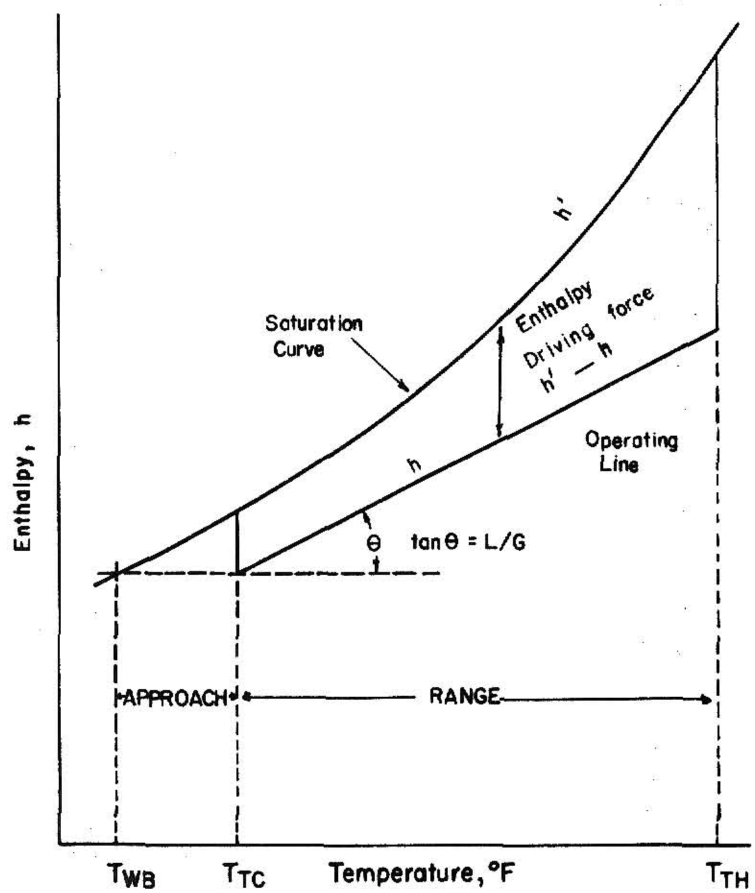
Then the tower unit can be expressed as

$$TU = K'a'V' \tag{3.5}$$

$$= W \int_{T_{TC}}^{T_{TH}} \frac{dT}{(h' - h)} \tag{3.6}$$

Figure 3-2 illustrates how the saturated enthalpy curve and operating line can be used to define the commonly used parameters, the wet bulb temperature T_{WB}, the entering temperature of the tower T_{TH}, the leaving temperature of the tower T_{TC}, the range, the approach, the slope of the operating line which is usually approximated by the liquid over gas flow rate L/G, and finally the driving force at any temperature, the difference between the enthalpy of saturated air and the enthalpy on the operating line.

In order to find the number of tower units, TU, the integral must be evaluated. In Fig. 3-3, a new graph is constructed with $1/(h' - h)$ vs. T. This curve is then integrated from T_{TC} to T_{TH}. This integration can be



Saturation curve and operating line
(Cooling Tower Institute, 1967).

Fig. 3-2. Representation of the wet bulb temperature, range, approach, operating line, and driving force on an enthalpy versus temperature diagram.

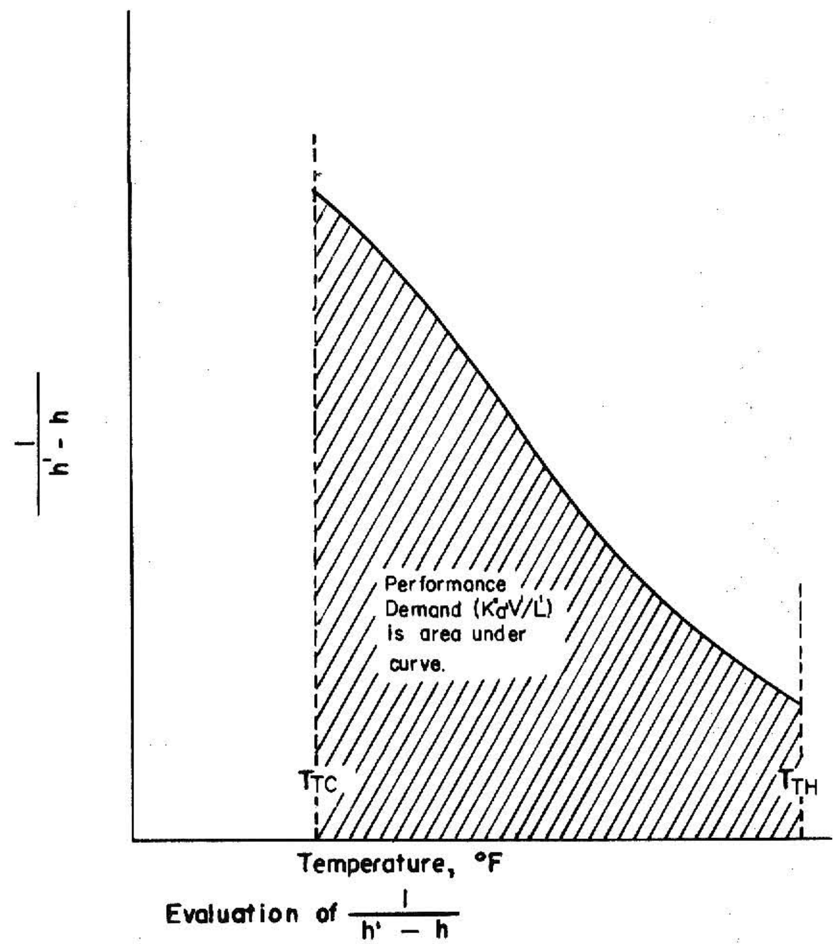


Fig. 3-3. Graphical evaluation of (K'aV'/L'). (Cooling Tower Institute, 1967).

approximated by the Tchebychoff method of numerical integration which uses the following formula:

$$\frac{K'a'V'}{W} = \int_{T_{TC}}^{T_{TH}} \frac{dT}{(h' - h)} \approx \frac{T_1 - T_2}{4}\left(\frac{1}{\Delta h_1} + \frac{1}{\Delta h_2} + \frac{1}{\Delta h_3} + \frac{1}{\Delta h_4}\right) \qquad (3.7)$$

where

Δh_1 = value of $(h' - h)$ at $T_{TC} + 0.1(T_{TH} - T_{TC})$

Δh_2 = value of $(h' - h)$ at $T_{TC} + 0.4(T_{TH} - T_{TC})$

Δh_3 = value of $(h' - h)$ at $T_{TC} + 0.6(T_{TH} - T_{TC})$

Δh_4 = value of $(h' - h)$ at $T_{TC} + 0.9(T_{TH} - T_{TC})$

This entire derivation depends on the Merkel equation (Kern, 1950). Several assumptions made in the development of that equation must be noted, as pointed out by Gurney (1966).

(i) evaporation is neglected

(ii) no resistance to mass transfer is used at the interface

(iii) the latent heat is assumed constant

(iv) the specific heat of water is unity

(v) the Lewis relationship is assumed equal to one for the water/air system

The enthalpy of the saturated air can be computed from the following equations (Himmelblau, 1967; Henley, 1959).

$$h'(T) = C_{pa}\,(T - T_o) + H[\ell_v - C_{pv}(T - 32)] \qquad (3.8)$$

where

T = temperature of air

C_{pa} = heat capacity of dry air = (0.240 Btu/lb_m °F)

C_{pv} = heat capacity of the vapor = (0.45 Btu/lb_m °F)

T_o = base temperature = 0°F

ℓ_v = heat of vaporization of the vapor = (1075 Btu/lb_m)

and

$$H = \frac{18\ P_{H_2O}}{29(PT - P_{H_2O})} \tag{3.9}$$

where

P_{H_2O} = vapor pressure of the water, atm

$= \exp\ [\bar{A} + B/T_K + C(T_K) + D\ \ln(T_K)]$

T_K = temperature, °K

$\bar{A}$ = 70.43469

B = -7362.698

C = 0.0069521

D = -9.0

The total initial capital expense of the tower as calculated by the Marley Company (Dickey, 1973) using an average L/G = 0.6 is then

$$\text{Tower Cost} = TU(\$/TU) \tag{3.10}$$

where

TU = (Flow Rate) (RF)

Flow Rate = flow of cooling water, gallon per minute

$$RF = \int_{T_{TC}}^{T_{TH}} \frac{dT}{(h' - h)}$$

The value of (\$/TU) includes the cost of motors, erection, concrete basin, pump, electric controls and wiring. This equation has been used by the Marley Company (Dickey, 1973) to preduct the total costs of cooling towers and has proven to be more accurate than cost estimates based on cost per water flow rate, cost per Btu per hour of heat exchanged, or cost per kilowatt of electric power generated.

Pond Initial Capital Cost

The cost of the pond is directly related to the cost of the land on which the pond is built and the excavation cost to build the pond. The excavation cost has been estimated at between 60 and 90 cents per cubic yard. The cost then to build a one acre pond five feet deep is between \$4840/acre and \$7260/acre. The cost of land is usually between \$500/acre and \$2000/acre. Thus the total cost of a pond per acre is between \$5000/acre and \$10,000/acre.

The cost of a pond is also related to the size of the pond, or the surface area. To calculate the surface area, we must consider an energy balance about the water flowing through the pond as illustrated by Fig. 3-4 (Dynatech, 1969; Tichenor and Christianson, 1971). The heat balance yields

$$q = \text{heat loss} = C_{pw}\rho_w(\text{flow rate})(T_{PH}-T_{PC}) \tag{3.11}$$

where

C_{pw} = heat capacity of the water

ρ_w = density of the water

The heat lost can also be computed by considering an overall heat transfer coefficient K. This yields

$$q = (K)(A)\left[\frac{(T_{PH} - T_E) - (T_{PC} - T_E)}{\ln\left(\frac{T_{PH} - T_E}{T_{PC} - T_E}\right)}\right] \tag{3.12}$$

where

A = the area of the pond

Thus

$$C_{pw}\rho_w(\text{Flow rate})(T_{PH} - T_{PC}) = K\,A\left[\frac{T_{PH} - T_{PC}}{\ln\left(\frac{T_{PH} - T_E}{T_{PC} - T_E}\right)}\right] \tag{3.13}$$

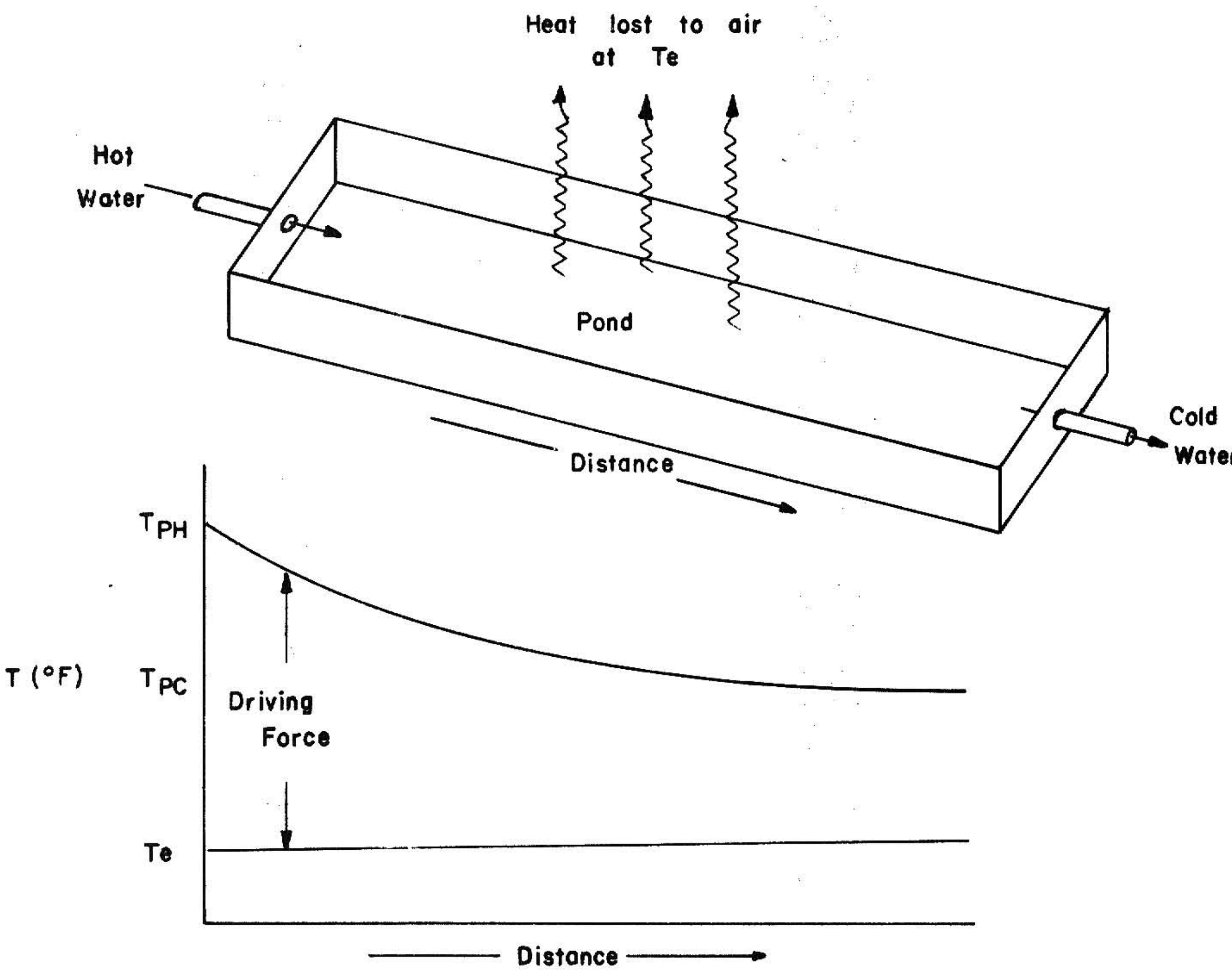


Fig. 3-4. Schematic representation of the cooling pond and temperature profile.

or

$$A = \frac{C_{pw}\rho_w(\text{Flow rate})}{K} \ln\left[\frac{T_{PH} - T_E}{T_{PC} - T_E}\right] \tag{3.14}$$

The total cost of the pond can be calculated by using the total cost of the pond per acre, "a", and the area of the pond, A, as follows;

$$\text{Pond Capital Cost} = a\,A \tag{3.15}$$

or

$$\text{Pond Capital Cost} = \frac{a(C_{pw}\ell_w)(\text{Flow rate})}{K} \ln\left[\frac{T_{PH} - T_E}{T_{PC} - T_E}\right] \tag{3.16}$$

Operating Costs

Operating costs for this system can be split into two types, the pumping cost and the fan operating cost. The pumping cost is assumed to be independent of the selection of the cooling pond or tower and is, therefore, charged to the power plant. Fig. 3-5 illustrates the reasoning behind this decision. Since similar heights and distances are used for the tower and the pond, equal weight should be given to either selection.

Two major pressure drops occur throughout the systems, one through the condenser and the other through the transportation line. The condenser is assumed to be a single pass shell tube heat exchanger with 4500 tubes 1 in. I.D., 12 ft. long. The transportation line is approximated by a section of 10, 2 ft. I.D. pipes 2000 ft. long with a height change of 30 ft., as in Fig. 3-4. The pressure drop is calculated as follows (Peters and Timmerhaus, 1968);

$$f = \text{friction factor} = \frac{0.04}{Re^{0.16}} \tag{3.17}$$

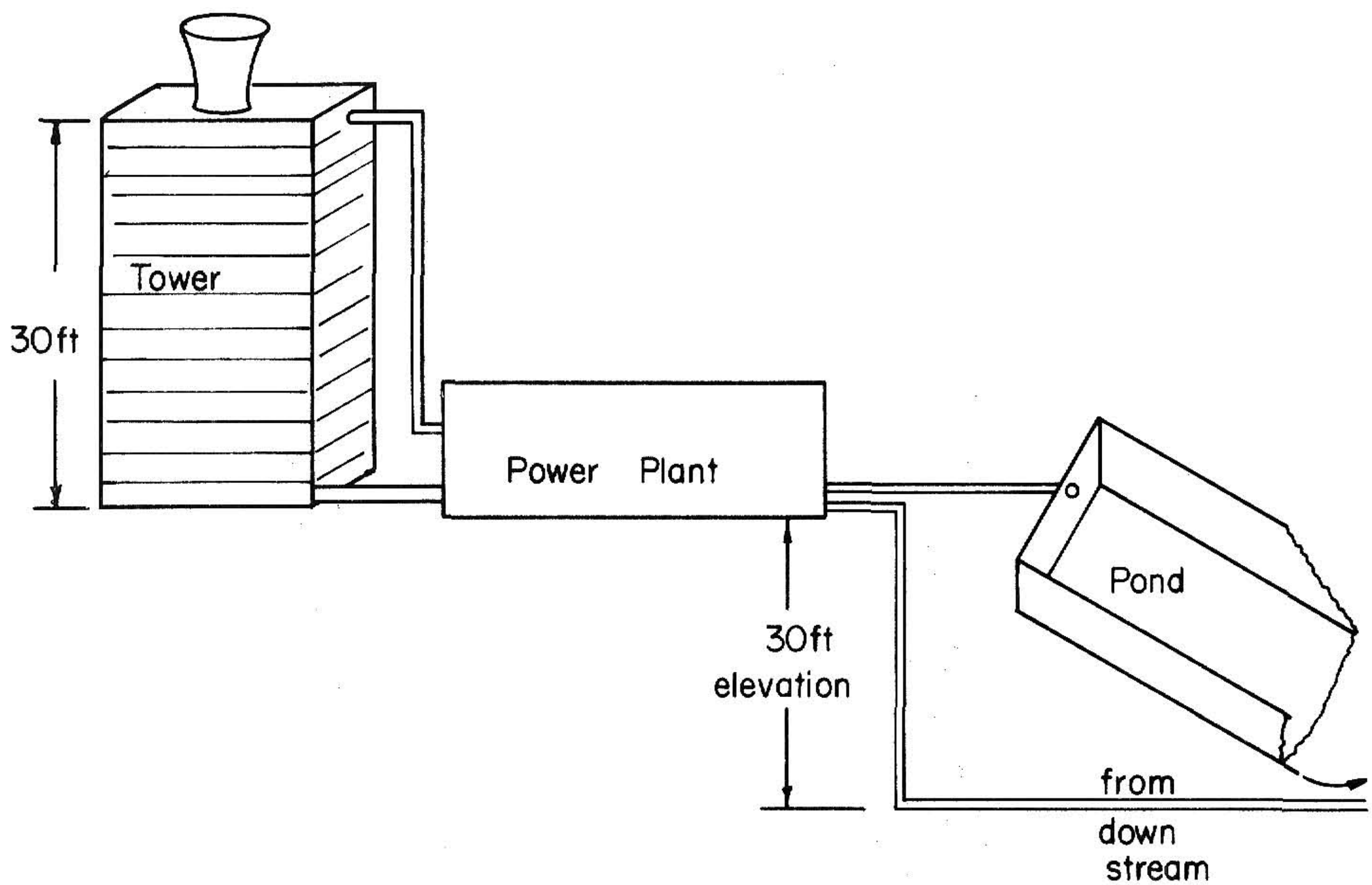


Fig. 3-5. A representation of the elevation differences of the subsystems in a cooling system.

$$\text{Pressure drop} = \sum_{i=1}^{2} \frac{2\, f_i\, V_i^2\, (L_i)}{g_c\, D_i} + 30 \text{ ft } lb_f/lb_m \tag{3.18}$$

where

i = 1 for the condenser

i = 2 for the transportation line

The pumping cost is then found as

$$\frac{\text{cost}}{\text{year}} = (\Delta P)\ \left(\frac{\text{hours}}{\text{year}}\right)\left(\frac{\$}{\text{Kwhr}}\right)\left(\frac{\text{hp}}{\Delta P}\right)\left(\frac{1}{\text{eff}}\right) \tag{3.19}$$

where

$\frac{\text{hours}}{\text{year}}$ = 8440 hours

$\frac{\$}{\text{Kwhr}}$ = \$0.01/Kwhr

eff. = pump efficiency

The second type of operating expense is the fan cost in the mechanical draft cooling tower. The Marley Company (Dickey, 1973) found that the ratio of the brake horse power needed to drive the fan motors over the number of tower units is a constant. Thus the operating costs for the fan can be calculated as

$$\text{fan operating costs} = \left(\frac{\text{Brake horsepower}}{\text{TU}}\right)(\text{TU})\left(\frac{\text{kwhr}}{\text{hr}}\right)\left(\frac{\$}{\text{kw}}\right)\left(\frac{\text{hours}}{\text{year}}\right) \tag{3.20}$$

SOLUTION METHOD

The optimal synthesis of cooling systems has been solved with two methods, the direct search, and dynamic programming.

Direct Search

In this approach, the following variables are fixed: the wet bulb temperature (75°F), the equilibrium temperature (80°F), cost of electricity (1¢/Kwhr), the heat exchanged from the condenser to the water (4.011×10^9 Btu/day), the Brake horsepower of the fan per tower unit (0.011 Bhp/TU), the density of water, the heat capacity of water, and the overall heat transfer coefficient of the pond (150 Btu/day ft^2 °F).

The structure of the integrated cooling system according to the structural parameter formulation is illustrated in Fig. 3-6. The various temperatures in the system, T_H, the temperature of the water leaving the condenser; T_{TH}, the temperature of the cooling water entering the tower; T_{TC}, the temperature of the water leaving the cooling tower; T_{PH}, the temperature entering the cooling pond; T_{PC}, the temperature leaving the cooling pond, and T_C, the temperature entering the condenser, are illustrated. The structural parameters $\alpha_{1,1}$, $\alpha_{2,1}$, $\alpha_{3,1}$, $\alpha_{1,2}$, and $\alpha_{3,2}$ are also indicated in Fig. 3-6.

The independent variables in the optimization procedure are T_C, T_{TC}, $\alpha_{2,1}$, $\alpha_{3,1}$, and $\alpha_{1,2}$. Since the temperature of the water entering the condenser, T_C, is an independent variable, the water flow rate through the condenser is a dependent variable. In order to bound the fluid velocity in the system, two constraints have been added.

$$\left.\begin{aligned} g_1 &= 10 - V_S \geq 0 \\ g_2 &= 10 - V_C \geq 0 \end{aligned}\right\} \qquad (3.21)$$

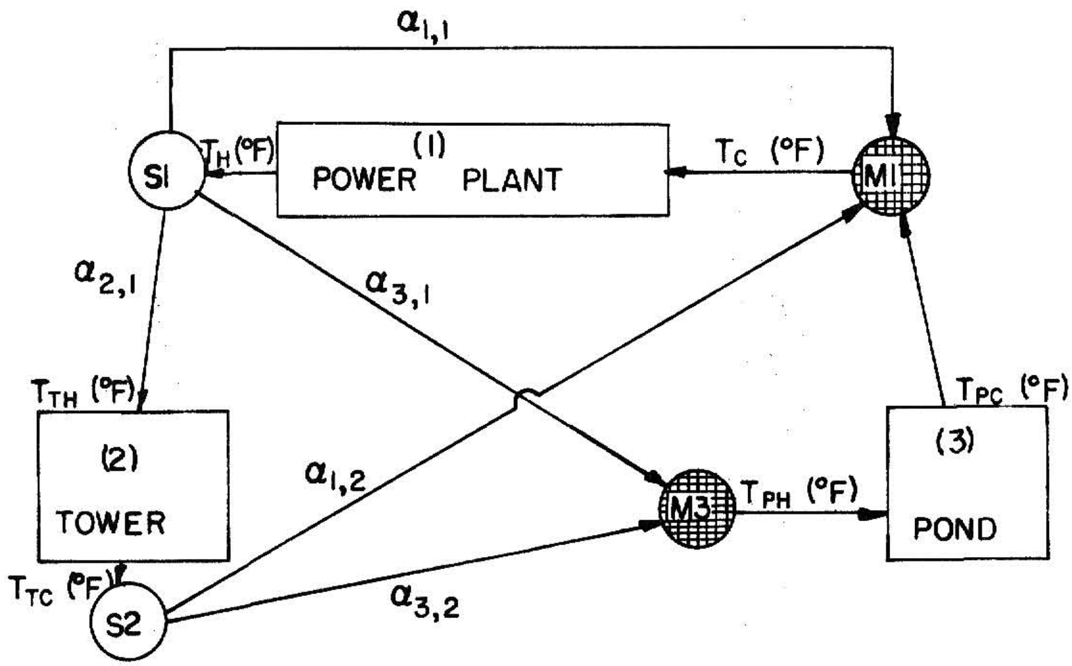


Fig. 3-6. The structure of the integrated cooling system according to the structural parameter solution formulation.

where

V_S = velocity in the transportation line

V_C = velocity in the condenser

The objective function is then

$$J = \text{OPCOST} + i_m \text{ (Tower cost + Pond cost)} \tag{3.22}$$

where

i_m = *minimum rate* of return is defined as the minimum acceptable return on the initial capital expense which includes a measure of the uncertainty of obtaining the desired profit.

OPCOST = operation cost of the pumps and fan, neglecting the cost of makeup water.

Thus the problem can be stated as

minimize: J

with respect to: T_{TC}, T_C, $\alpha_{2,1}$, $\alpha_{3,1}$, $\alpha_{1,2}$

such that g_1, $g_2 \geq 0$

The optimal solutions were found by using a sequential random search developed by Chen and Fan (1975).

Dynamic Programming

The basis for this approach is Bellman's (1957) "Principle of Optimality". It states "an *optimal policy has the property that whatever the* initial state and decision are, the remaining decisions must constitute an optimal policy with regard to the stage resulting from the first decision". Thus this method attempts to proceed through the final stage to the end of the process in an optimal manner with respect to the independent variable associated with the final stage. Next the optimal path through the next to last stage to the end of the process (utilizing information about the optimal path through the last stage found in the previous step) is found with respect to the independent variable associated with the next to last stage. These steps are repeated until the optimal path through the beginning stage to the end of the process if found.

The optimal synthesis of the cooling system can be achieved by considering the cooling process as a staged process. Temperature, in this approach, became a state variable and the changes in temperature are classified as stages. Fig. 3-7 is a representation of the dynamic programming solution to the cooling systems synthesis under consideration. As indicated in Fig. 3-7, the minimum temperature range is considered to be 10°F. Three stages are then needed to simulate the cooling process from 115°F to 85°F.

Figure 3-8 illustrates the identification of a stage and decision variable in the Dynamic Programming approach to the cooling system synthesis. As indicated in Fig. 3-8, the independent variable for each stage, the decision variable, is the splitting fraction of the flow of cooling water (structural parameter) which is diverted to the cooling tower.

Application of the principle of optimality to the system under consideration yields the following recursive equation.

$$f_i(S_{i+1}) = \min_{\{\Theta_i\}}[g_i(\Theta_i, S_{i+1}) + f_{i-1}(S_i)] \quad (3.23)$$

where

$$f_0(S_1) = 0$$

$$i = 1, 2, 3$$

$$\begin{aligned} g_i(\Theta_i, S_{i+1}) = {} & \Theta_i[\text{Tower Operating Cost } (S_{i+1}, S_i)] \\ & + i_m\{\Theta_i[\text{Tower Capital Cost } (S_{i+1}, S_i)] \\ & + (1 - \Theta_i)[\text{Pond Capital Cost } (S_{i+1}, S_i)]\} \end{aligned} \quad (3.24)$$

In these expressions

i_m = minimum rate of return

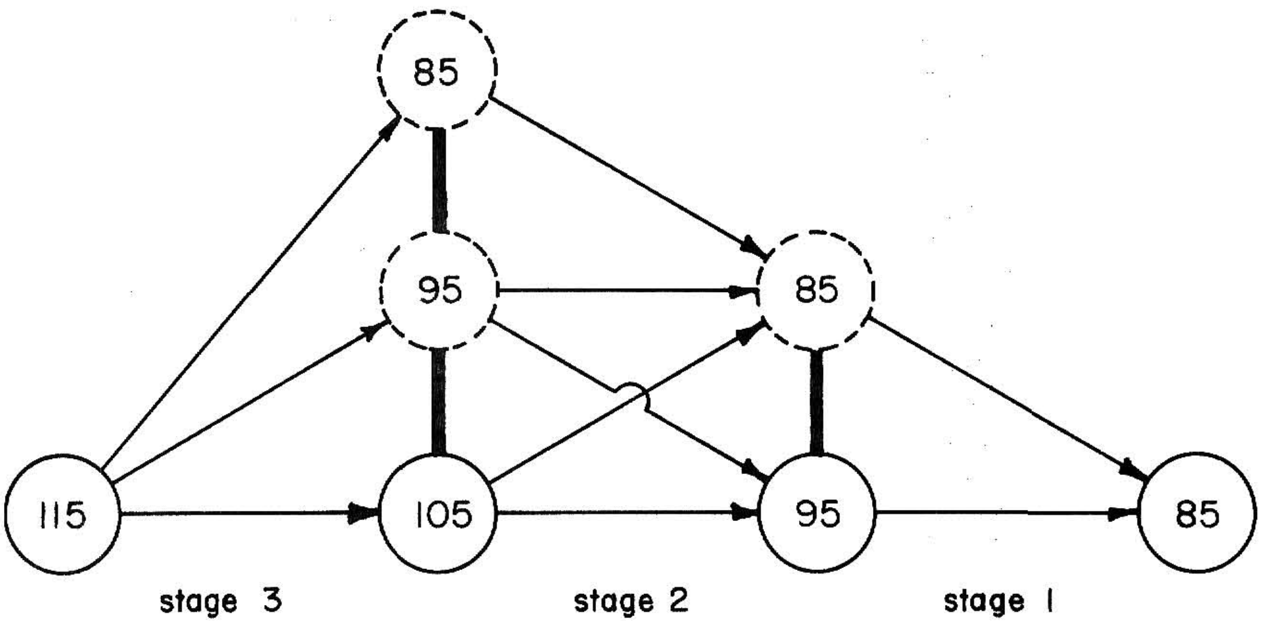
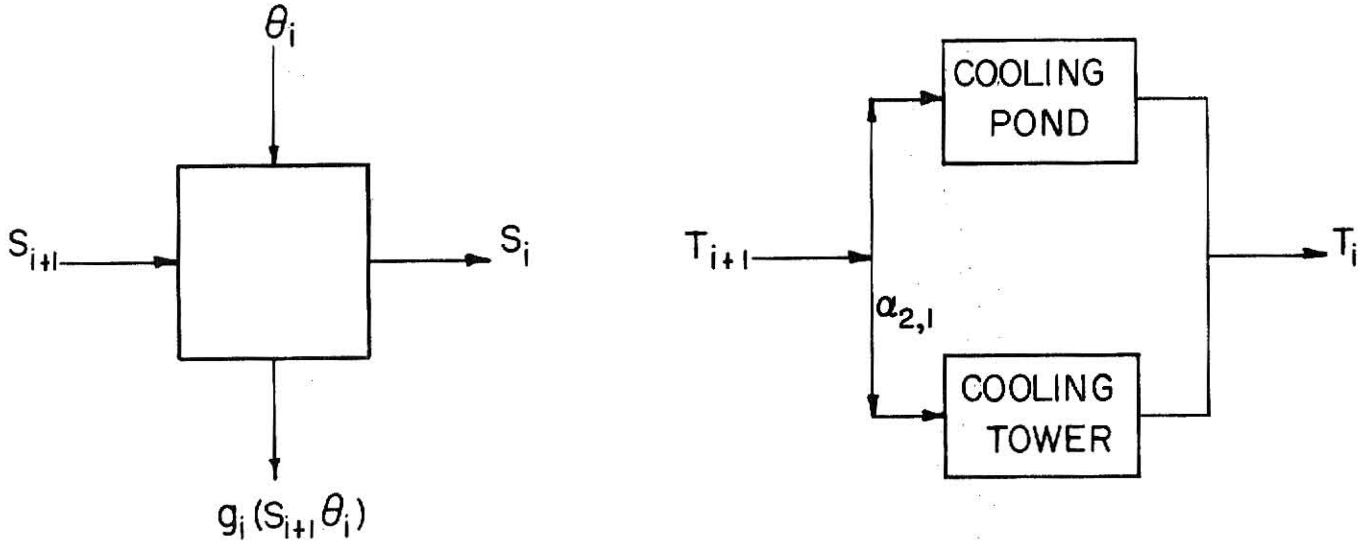


Fig 3-7. Schematic representation of the dynamic programming solution of cooling system synthesis.



$$\theta_i = \alpha_{2,1}$$
$$S_{i+1} = T_{i+1}$$
$$S_i = T_i$$

Fig. 3-8. Identification of stage and decision variable in the dynamic programming approach to the cooling system synthesis.

$$\text{Tower Capital Cost } (S_{i+1}, S_i) = (\frac{\$}{TU})(TU) \tag{3.25}$$

where

$$TU = (\text{Flow Rate})[\int_{S_i}^{S_{i+1}} \frac{dS_i}{(h' - h)}]$$

TU = tower unit

$$\text{Pond Capital Cost } (S_{i+1}, S_i) = a\frac{(C_{pw}\rho_w)(\text{Flow rate})}{K} \ln[\frac{(S_{i+1}-T_E)}{(S_i-T_E)}] \tag{3.26}$$

where

ρ_w = density of water

a = land cost per acre

C_{pw} = heat capacity of water

K = overall heat transfer coefficient

T_E = equilibrium temperature

$$\text{Tower Operating Cost } (S_{i+1}, S_i) = (TU)(\frac{BHp}{TU})(\frac{Kwhr}{hrhp})(\frac{\$}{Kwhr})(\frac{hr}{year}) \tag{3.27}$$

The optimal solution is obtained by repeatedly applying the basic recursive equation to each stage, beginning at stage 1 (the last stage).

$$f_1(S_2) = \min_{\{\Theta_1\}}[g_1(S_2, \Theta_1) + f_o(S_1)]. \tag{3.28}$$

where

$$f_o(S_1) = 0$$

$$f_1(S_2) = \min_{\{\Theta_1\}}[g_1(S_2, \Theta_1)]$$

$$f_2(S_3) = \min_{\{\Theta_2\}}[g_2(S_3, \Theta_2) + f_1(S_2)] \tag{3.29}$$

$$f_3(S_4) = \min_{\{\Theta_3\}}[g_3(S_4,\Theta_3) + f_2(S_3)] \tag{3.30}$$

The dynamic programming solution presented above has only three stages because the minimum temperature range is considered to be 10°F and the beginning and end states are 115°F and 85°F respectively. The number of stages could then be increased if the temperature range in each stage is decreased.

RESULTS AND DISCUSSION

The results are presented and analyzed in this subsection. The advantages and disadvantages and various other facets of each of the methods used and other available synthesis methods are then discussed.

Direct Search

The minimum rate of return, i_m, temperature leaving the condenser, T_H, and the ratio of the pond cost per acre to the cost of the tower per tower unit, $\frac{TU}{Acre}$, are all parameters that are adjusted in order to judge their importance.

All of the resulting optimal structures have the following values for indicated independent and dependent variables.

$\alpha_{1,2} = 0$

$\alpha_{2,1} = 1$

$\alpha_{3,1} = 0$

$\alpha_{1,1} = 0$

$\alpha_{3,2} = 1$

The resulting system structure, as shown in Fig. 3-9, is a series combination of the tower and pond. The optimal structures were variations on this reduced system. Three of the parameters used in the model were adjusted to determine the relative importance of each. The three parameters that were adjusted were r, T_H and i_m.

In Fan and Lin's (1975) formulation of the cooling system design, the cost parameters for the tower costs were completely empirical parameters. The cooling tower cost was correlated to the amount of heat removed. Eighteen cooling towers were used to develop the cost correlation.

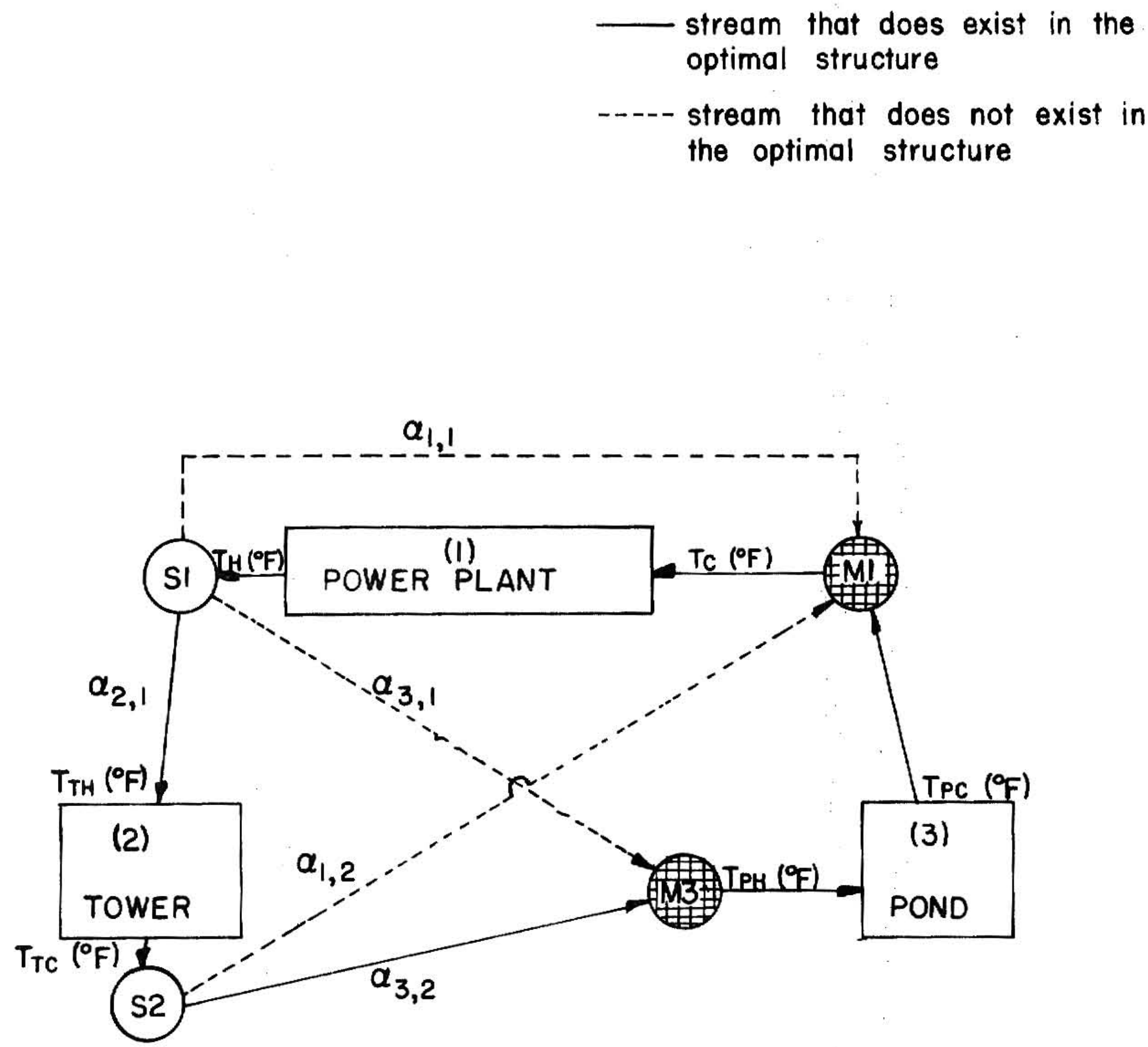


Fig. 3-9 The series combination of the tower and the pond resulting from the optimal solution by the direct search.

The tower unit cost equation has an advantage that the economic and the heat transfer portions of the cost equation can be easily separated. The number of tower units, TU, and the cost of a tower unit, (\$/TU), are definitely distinguishable. The number of tower units, TU, needed for a cooling tower is dependent only on the amount of heat that must be removed, and the thermal conditions of the proposed cooling tower and cooling tower sight, wet bulb temperature, T_{WB}, temperature entering the tower, T_{TH}, and the cold water temperature leaving the tower, T_{TC}.

The cost of a tower unit, (\$/TU), is only dependent on the present economic condition, cost of material and cost of labor. Therefore, the cost of a cooling tower relative to some other cooling unit, a cooling pond, can be precisely calculated by using the parameter r which is defined as the ratio of the cost of the cooling pond, a, to the cost of the cost tower per tower unit (\$/TU).

It can then heuristically be thought of as a measure of the number of tower units that are equivalent to an acre of pond under a set of economic conditions. Figure 3-10 plots the fraction of the initial capital expense used on the pond and Fig. 3-11, the annual cost vs. r. As in Fan and Lin's work, the results indicate that at some low land cost, the pond will predominate and the optimal design will only have a single pond. At some large value of r the tower will predominate. As indicated in both figures, however, there is a region of r values at which the optimum configuration is a combination of the pond and tower. The result of the present work differs from that of Fan and Lin's (1975) since they found only homogeneous systems optimal because of the linearized objective function. This result agrees with the results of Gupta (1973). Gupta found that a heterogeneous combination of a dry mechanical draft pond system was optimal.

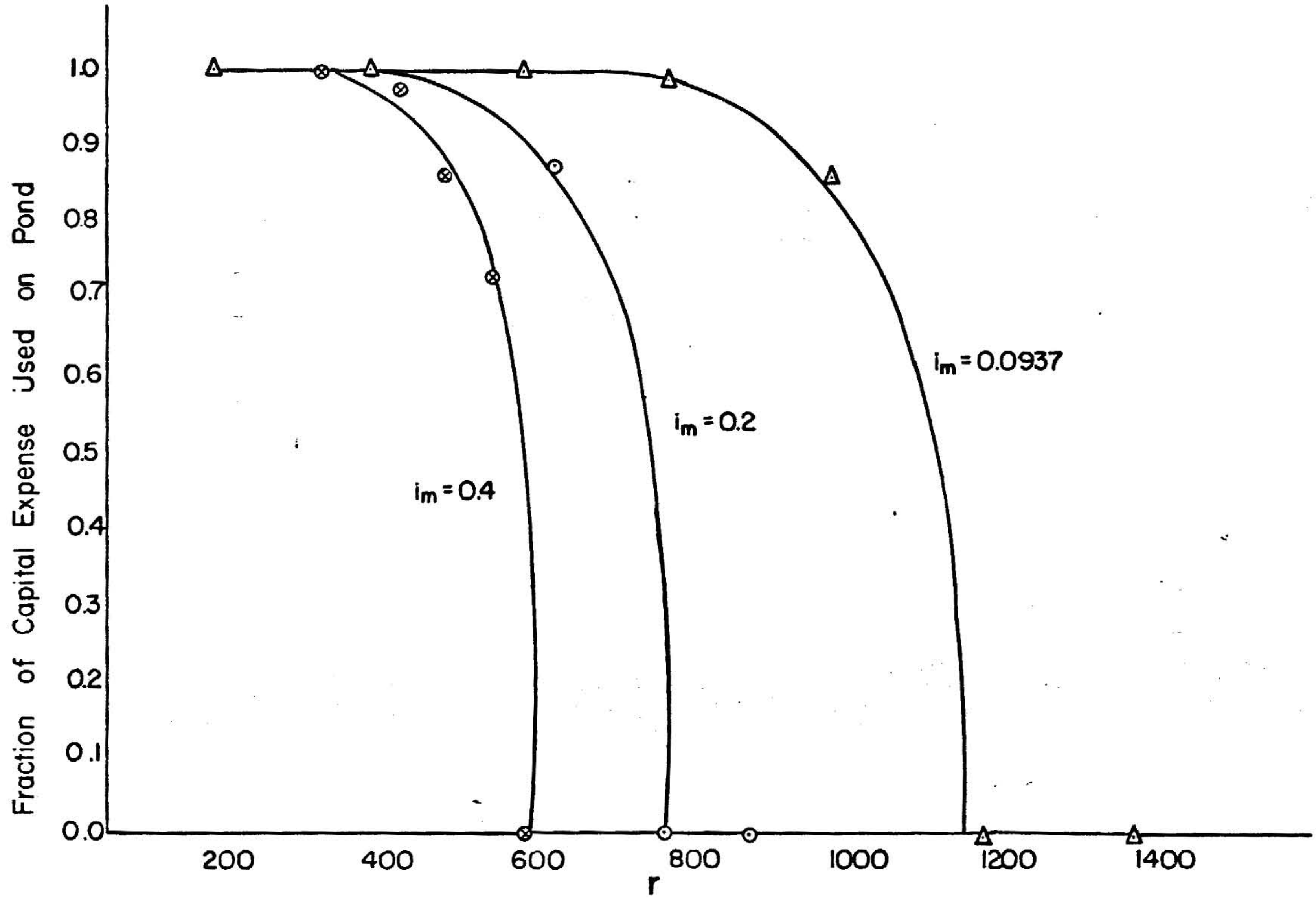


Fig. 3-10. Fraction of capital expense used on pond vs. r.

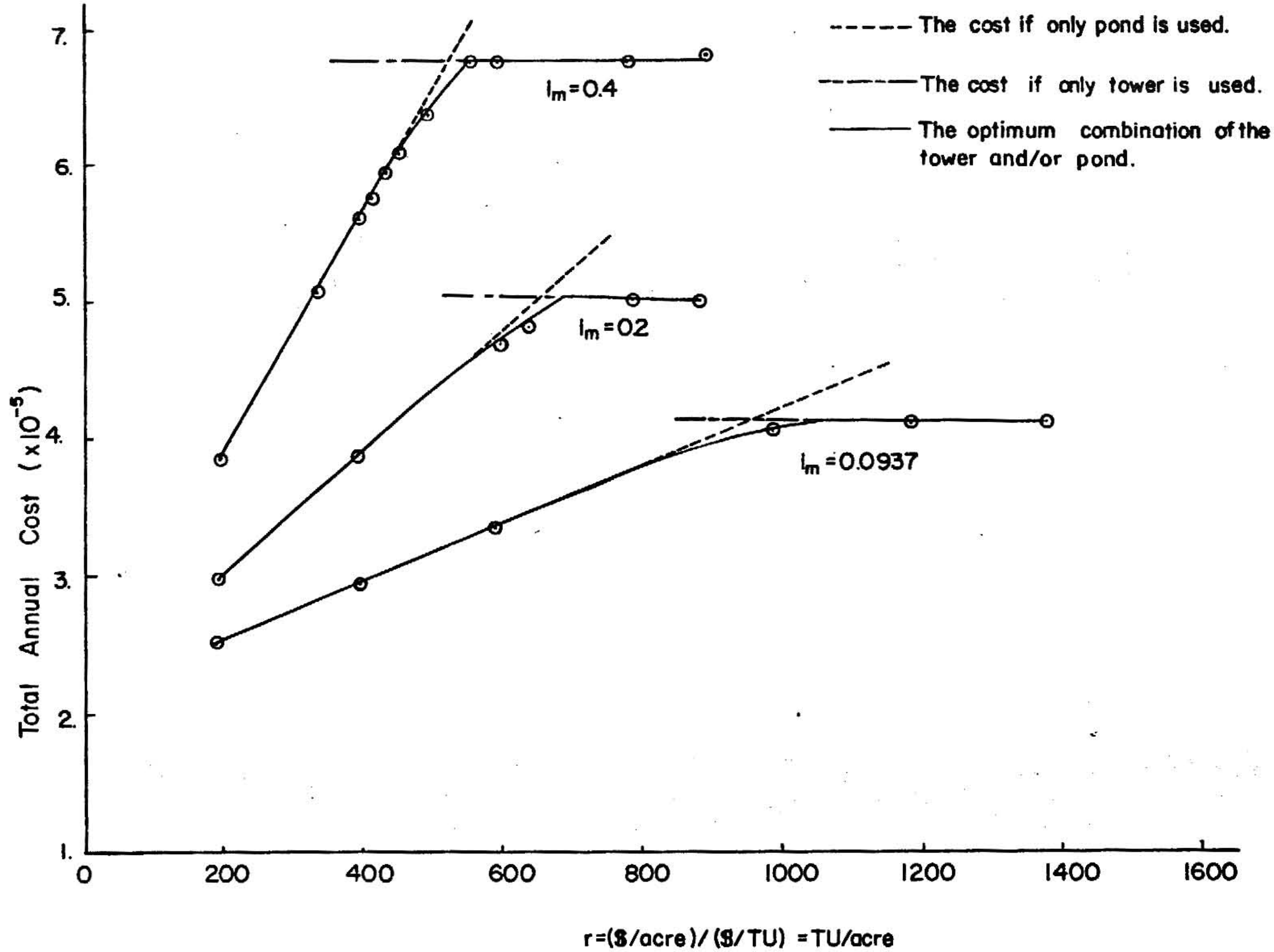


Fig. 3-11. Total annual cost (x10^{-5}) vs. r with i_m as a parameter.

Figure 3-12 plots the temperature of the water leaving the tower and entering the pond. As before, this temperature indicates the effect of the parameter, r.

The effect of the minimum rate of return, i_m, is then shown in Figs. 3-10, 3-11, and 3-12. The minimum rate of return, i_m, is the minimum return on the initial capital expense that can be expected on the investment. If a proposed project is very risky, the expected risk can be offset by increasing the minimum rate of return which causes a decrease in the profit function to account for the risk. Since the pond has a small operation expense compared to the tower, when more weight is given to the operating expense, the tower is favored and the curve shifts to the left on the annual cost vs. r plot. The curve also shifts upward due to the increase in capital expense charged to the annual costs.

A minimum rate of return, i_m, can also be interpreted as a conversion factor used to convert an initial cost to an annual cost, a unacost. By using this interpretation, i_m then becomes a present worth to the unacost factor. For example, on Figs. 3-10, 3-11, and 3-12, $i_m = 0.0937$ is the present worth to unacost factor for a system with a lifetime of twenty-five years with a constant annual rate of interest of 8% as indicated by Jelen (1968).

Since the hot temperature leaving the condenser has been fixed through the study, its effect is also checked. Figure 3-13 plots the annual cost vs. r for two different temperatures. Since the water flow rate is a function of the heat exchange, the area available for heat transfer, the overall heat transfer coefficient, and the temperature difference, the flow rate will most certainly change. All of these facts except the temperature difference are fixed in this problem so that the flow rate of water will

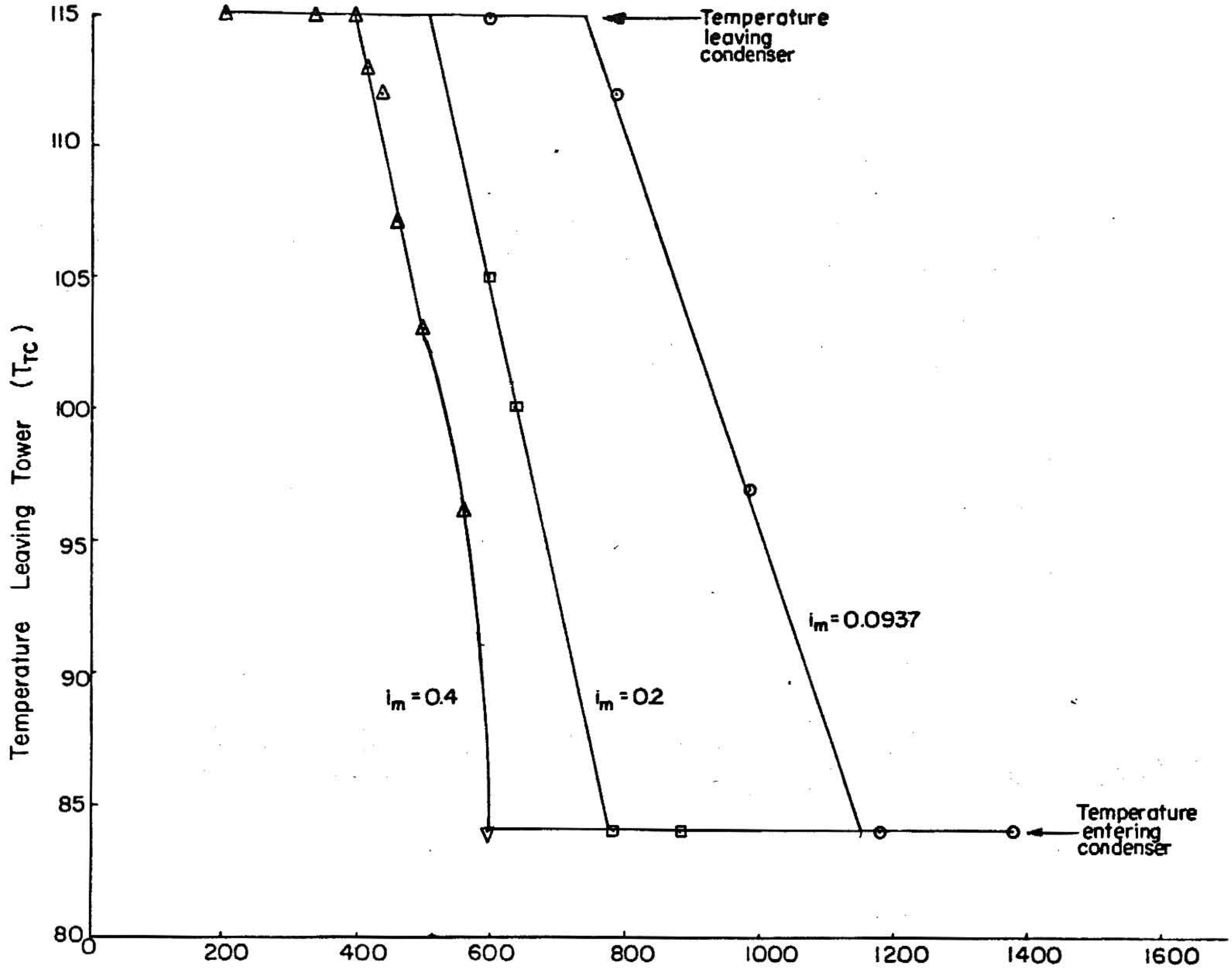


Fig. 3-12. The temperature leaving the cooling tower.

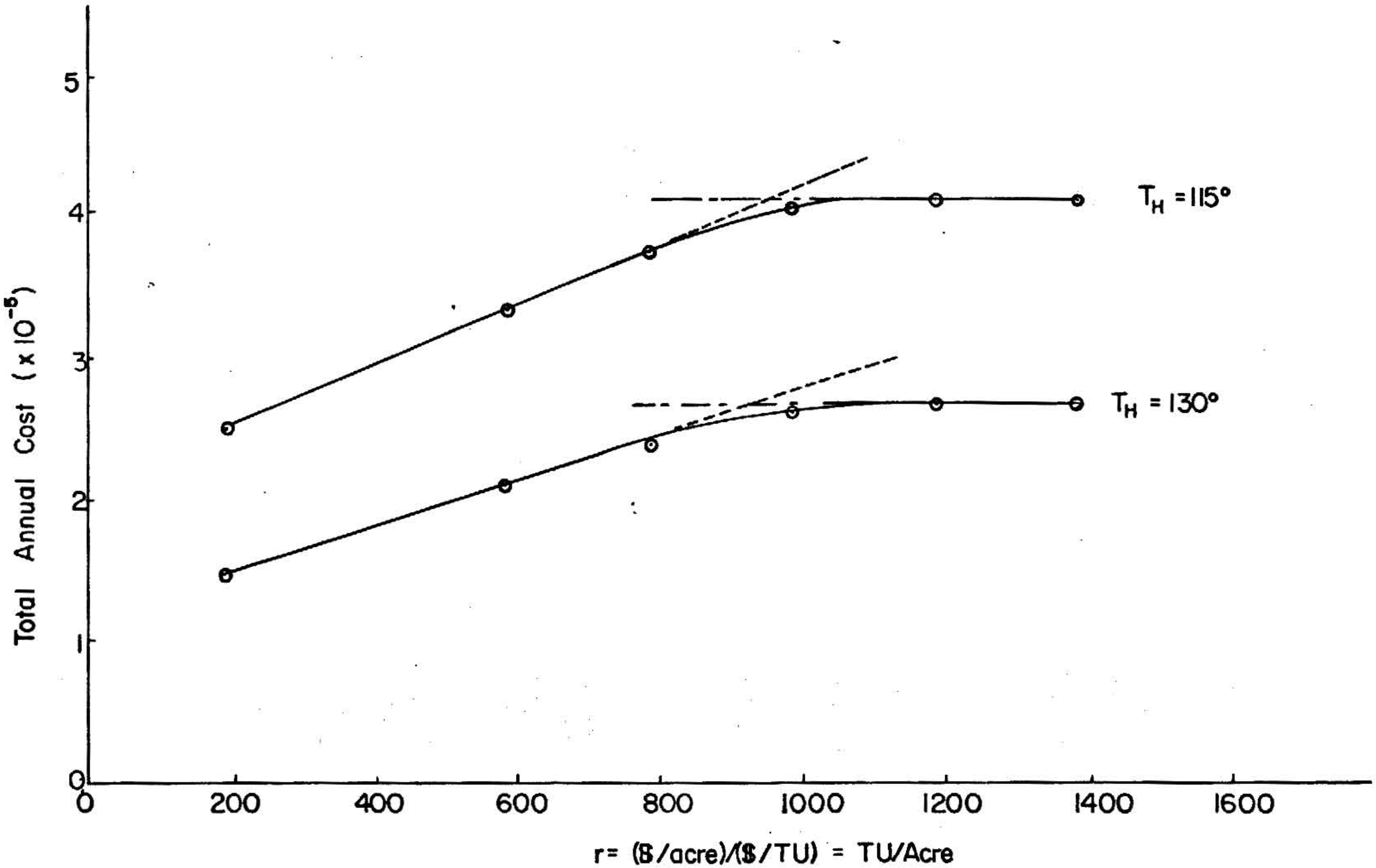


Fig. 3-13. Total annual cost ($x\ 10^{-5}$) vs. r .

be reduced directly when the temperature difference is increased. The annual cost will then decrease because of a decreased flow rate.

The savings achieved with a heterogeneous system as indicated by Fig. 3-14 are small with respect to the homogeneous system with a pond only. They are on the order of only \$7,500/year when the total annual costs are on the order of \$400,000/year. These savings of only 2.0% force one to choose a heterogeneous system must be more closely examined. This paper has not added the additional operating expenses of labor associated with each unit. One might expect a higher labor cost for the tower unit than for the pond. This paper has not added a cost for make up water, since it was assumed this plant would be in a low cost water area. But the savings associated with the correct choice of a pond or a tower in the regions of r beyond and below the region of the optimal heterogeneous system are large. For example, perhaps a system has a pond cost of \$5,000/ acre and a \$/TU cost of \$5/TU, then either the pond or tower would give similar annual costs for $i_m = 0.0936$. However, what if the \$/TU cost then shifted due to economic reasons to \$6.25/TU. The r would be 800 and the pond for $i_m = 0.0937$ would be by far the most suitable choice. The pond would be on the order of \$35,000/year or about 9% of the total annual cost cheaper.

Dynamic Programming

Table 3.1 contains the optimal results obtained by means of equation (3.28) for stage 1. Table 3.2 contains the results obtained by means of equation (3.29) and Table 3.1 for stages 1 and 2. Table 3.3 contains the results obtained by means of equation (3.30) and Table 3.2 for stages 1, 2, and 3.

Through examination of the optimal Θ_i at each stage, the optimal path throughout the system can be determined. The physical interpretation of

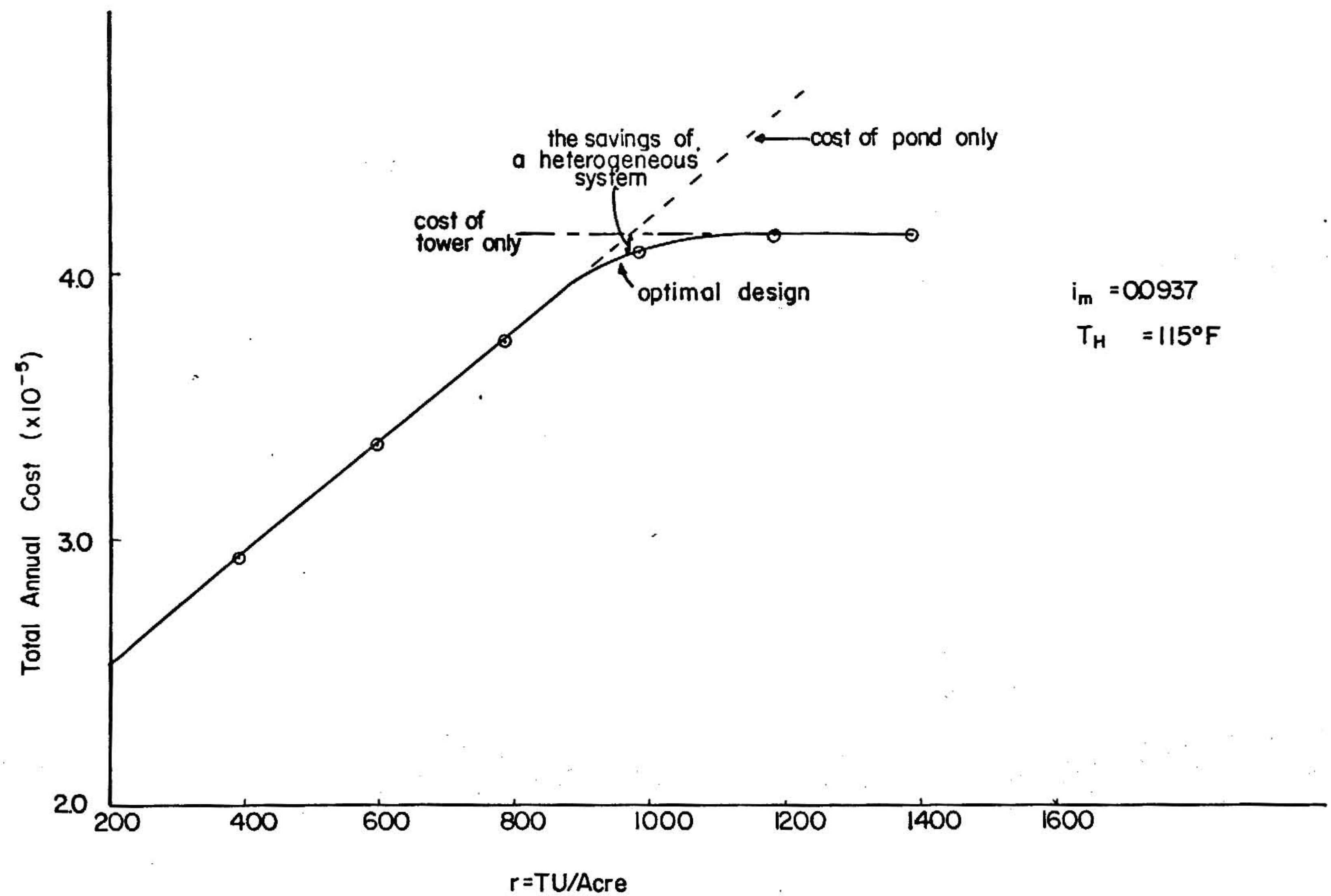


Fig. 3-14. The savings of a heterogeneous system over homogeneous system.

TABLE 3.1

S_2	$f_1(S_2)$	S_1	Θ_1
95	90,974.90	85	0
85	0	85	--

The Optimal Results of the

Dynamic Programming Procedure for Stage 1.

TABLE 3.2

S_3	θ_2	S_2	g_2	f_1	f_2
105	0.0	95	42300.80	90974.90	133275.3
105	0.0	85	133275.3	0	133275.3
95	---	95	0	90974.90	90974.90

The Optimal Result of the

Dynamic Programming Procedure for Stage 2.

TABLE 3.3

S_4	θ_3	S_3	g_3	f_2	f_3
115	1.0	105	26,459.28	133,275.30	159739.58

The Optimal Results for the

Dynamic Programming Procedure for Stage 3.

the optimal design is a cooling tower from 115°F to 105°F and a cooling pond from 105°F to 85°F. A savings of $1403.80/year is obtained by using the resulting heterogeneous system instead of using either a homogeneous cooling pond or tower system. It has been found that, for every case, the structure has been a series structure and the cooling tower is always on the hot end of the temperature range. This fact means that, with two single variable optimizations, it is possible to determine the existence of a heterogeneous system. The proposed method would begin by finding the cheapest way to proceed through the first stage. Next find the cheapest way to proceed through the final stage. If the heat transfer units generated are different, then the system must be further optimized with the procedure defined in the earlier section in order to determine the temperature between the respective units. If the heat transfer units are the same for the two test cases, then the system will be homogeneous.

The accuracy and the computational effort of the dynamic programming method are dependent on the size of the temperature range in a stage. A reduction in the temperature difference cause additional stages to be required and also additional computational effort is needed. If a large temperature difference is used, the intermediate temperature between different cooling subsystems is not accurately defined.

A procedure used in the dynamic programming method is to first find an approximate optimal solution. This approximate solution is used to develop a more exact optimal solution that does not require excessive computations. This method of iteratively generating more exact solutions can produce very exact solutions without excessive computational effort.

The intermediate temperature between the cooling tower and pond can be found by using an iterative procedure by first using the 10° range in each stage, as explained in the earlier pages. The result is that a cooling pond is used on the cooler end of the cooling range and a cooling tower is used on the hotter end of the cooling range. The temperature between these two units is first approximated at 105°F. In order to determine this temperature more exactly a second iteration of the dynamic programming procedure is used. Since the first iteration has determined that the pond is on the cool end and the tower is on the hot end of the cooling range, the next iteration must only examine the middle portion of the cooling range. For the second iteration the cooling considered will be from 100°F to 110°F. A two stage process will be considered, Stage 1 (105 to 100°F) and Stage 2 (110 to 105°F). The dynamic programming solution to this second iteration will then determine the intermediate temperature between the cooling tower and cooling pond more exactly. This process can be repeated indefinitely to increase the accuracy of the intermediate temperature between the cooling units.

If the iterative procedure above were not used, and a smaller temperature range was used for each stage, the number of stages needed would be six and thus the complexity of the dynamic programming solution would be greatly increased as indicated in Fig. 3-15.

The method used by Gupta (1973) to solve the dry cooling tower and cooling pond problem was a single variable search with only one problem to solve. The assumptions used in this approach is that the dry cooling tower will always be used on the hot side of the temperature range, and that only series systems were optimal.

The dynamic programming procedure used on the example problem solved in this paper does not make either of these assumptions. This method can also be used to generate optimal cooling systems with dry cooling towers, wet cooling towers, or cooling ponds by only using a three unit parallel subsystem instead of a two unit subsystem used in this example problem.

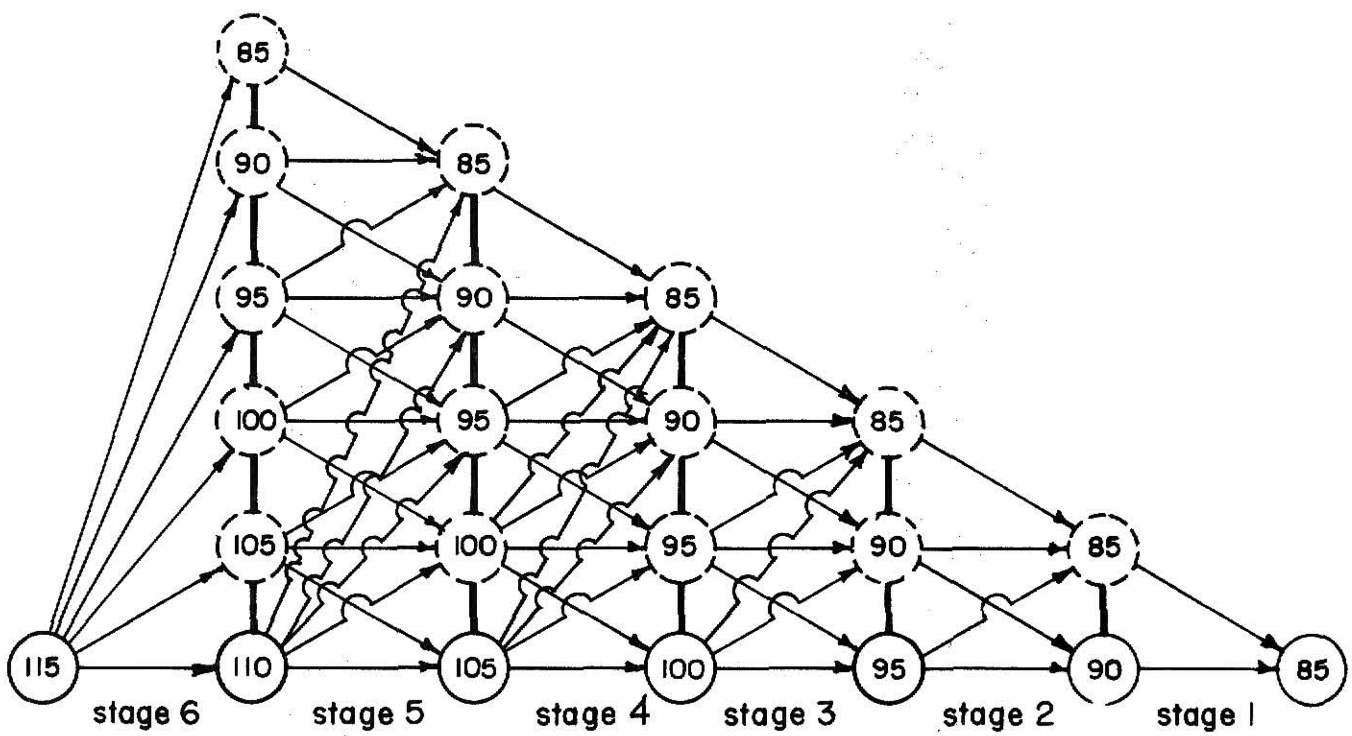


Fig. 3-15. Representation of the dynamic programming solution to the cooling system synthesis with the temperature range over each stage at 5°F.

Decomposition

The decomposition as proposed by Osakada and Fan (1972) or Umeda and Ichikawa (1972) can be applied to the cooling systems design. Starting from the integrated system in Fig. 3-16, a decomposed set subsystems was developed and is shown in Fig. 3-17. It should be noted that the original system has four independent variables and it is decomposed into a set of subproblems, two variable problems and one recombination problem of six variables. As noted in the section on decomposition methods as applied to system synthesis, this problem would take less computer space than the larger problem, but the decomposed problem will take more time than the combined, non-decomposed problem.

Umeda, Shindo, and Tazaki's (1972) method of feasible decomposition will not work with this problem since the number of independent variables is less than the number of coordination variables.

Evolutionary Approach

An evolutionary approach can also be used to design the cooling system. As described in the earlier section on evolutionary optimization, the method consists of first starting with a basic design. The assumed design is optimized and the results are examined to determine a structural change that will cause an increase in profit or a decrease in cost. If a structural change can be identified, then the change is incorporated in the design and the new system is reoptimized. This technique can be repeated until no new designs can be generated.

Evolutionary techniques, when applied to cooling systems synthesis, will reduce to first picking any type of cooling unit, a tower or a pond. Next a different type of unit is incorporated into the design and the system is reoptimized. For example, consider the original design to be a wet mechanical draft cooling water tower with the TU/acre equal to 800. The temperature of the hot stream entering the cooling system is 115°F. The

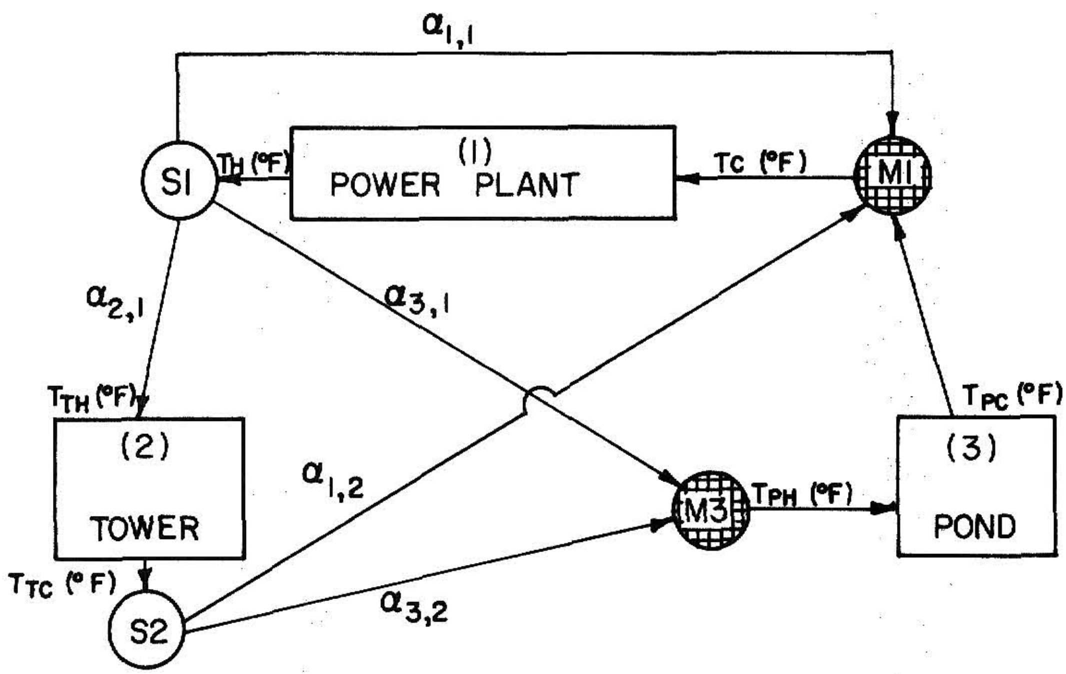


Fig. 3-16. The structure of the integrated cooling system according to the structural parameter solution formulation before decomposition.

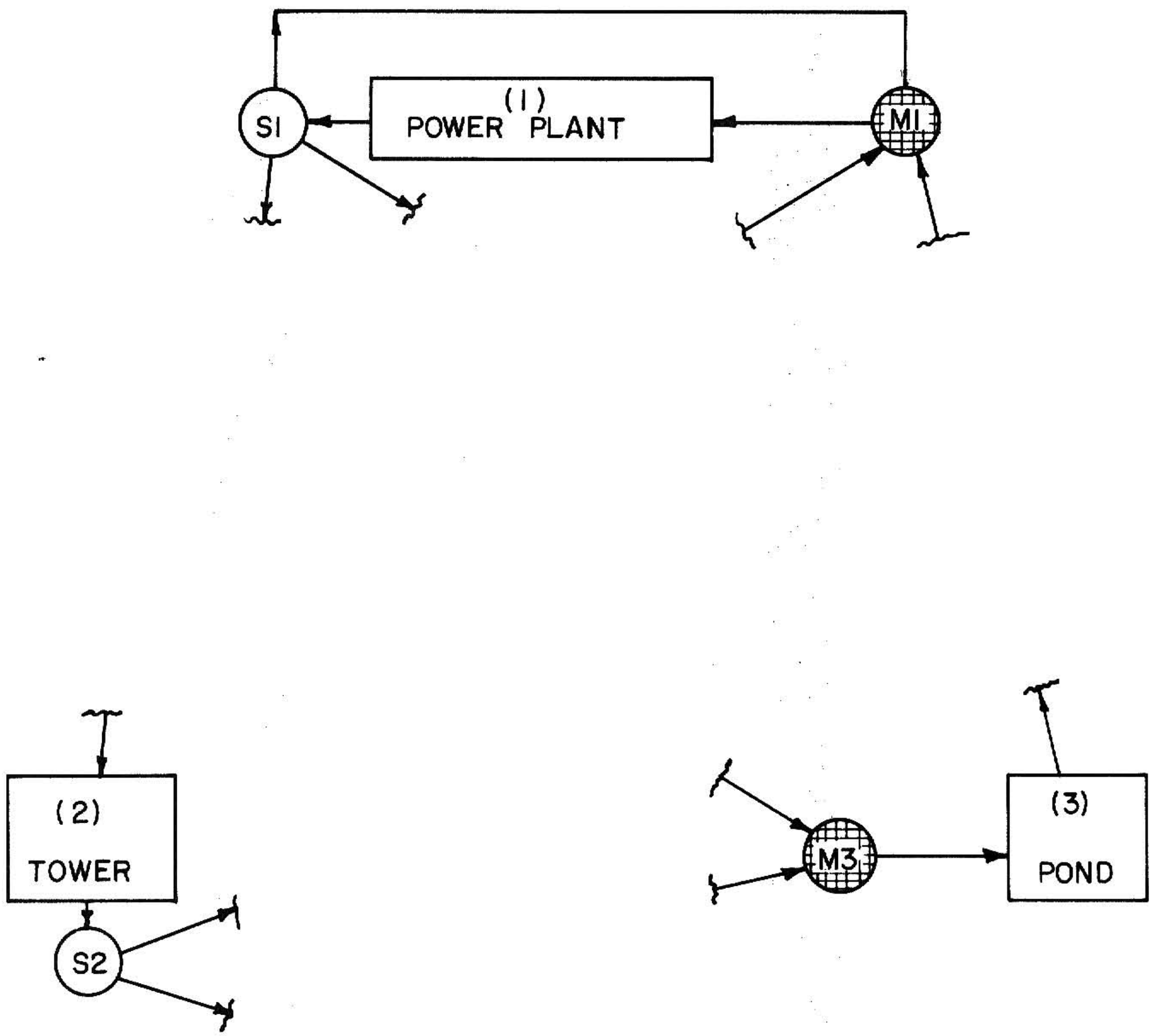


Fig. 3-17. A representation of decomposed cooling system.

minimum rate of return is 0.0937. With this simple a system, no optimization is needed. Next, the cost comparison is made between the cooling tower and the pond. The tower will cost about \$4.2 x 10^5 per year. No further optimization is needed. The design then becomes a cooling system with a pond instead of a tower.

With this problem, the system is so simple that evolutionary approach's true potential is not realized. For a larger system, such as the second example in this thesis, the design of a two reactor, two distillation column problem, the practicality of using evolutionary optimization becomes more apparent.

Other Techniques

Since a heat exchanger and a cooling system for a power system accomplish the same job, one would expect that those synthesis techniques used in heat exchanger design could be used for cooling system design. The problem is that, usually in exchanger network synthesis, the number of hot and cold streams is at least greater than four. In cooling systems synthesis, there is only one hot stream and one cold stream, the atmosphere. In addition, in heat exchanger synthesis, only homogeneous units are considered, but in cooling system design, the selection of the units is the basic problem. Therefore, neither the branch and bound nor the feasible matrix, decision tree algorithm can be used in cooling system design as presently formulated.

A linear approach was used by Fan and Lin (1974) to design cooling systems, but of course, according to his formulation of the problem, the objective function was linear. In this work, the objective function was not linear. In addition, the purpose of the paper is to investigate the applications of systems techniques to industrial problems and most industrial problems cannot, in general, be linearized. Linear simplifications and methods have been ignored.

As stated in Chapter 2, theorem proving cannot be used as a method in optimal systems synthesis until the application of, and the control of, the economic problem have been considered.

The heuristic technique might be very applicable in this cooling system problem. This paper has not considered this technique because the various heuristics needed in this problem were not readily available and the accuracy of the possible heuristics could not be determined until after the fact, after an optimal system was synthesized.

CONCLUSION

The optimal design of a cooling system is most directly affected by the ratio r, the ratio of the cost of land versus the cost of a tower unit. Optimal systems can be generated that are heterogeneous series systems for intermediate values of r. The savings associated with heterogeneous systems are small over similar homogeneous systems.

How the initial capital expense and the operating expenses are combined is a critical point, since the operating expense is not the same for different units. Relatively small changes in the i_m, the minimum rate of return, can influence the optimal homogeneous unit selection.

The temperature leaving the condenser in this study has little effect on the optimal unit selection. But the absolute value of the annual cost is affected.

From this study, Fan and Lin's (1975) work, Gupta's paper, and with the addition of the condenser design and natural draft tower consideration, the ultimate synthesis of a cooling system may be undertaken.

NOTATION	COMPUTER VARIABLE	
a'	--	surface area per cubic foot of packing (ft^2/ft^3)
a	--	cost of pond per acre
A'	A'	cross sectional area of tower (ft^2)
$\bar{A},B,C,D$	--	constants in vapor pressure equation
C_{pa}	--	heat capacity of dry air
C_{pv}	--	heat capacity of vapor
C_{pw}	CPW	heat capacity of water ($Btu/lb_m{}^\circ F$)
f	--	friction factor
$f_{i,j}$	--	suboptimal cost of cooling water from T_i to T_j; $j=1,2,3$, $i=j+1$
$f_{i,j}$	--	optimal combination of suboptimal processes $\sum_{K=i+1}^{j} f_{i,K}$, $j=1,2,3$
G	--	water mass flowrate (lb_{mole}/hr)
g_i	--	constraint i, $i = 1,2$
h	H(T)	enthalpy of air
h'	HS(T)	enthalpy of saturated air
h_1	H1	enthalpy of air entering tower (Btu/lb_m)
h_2	H2	enthalpy of air leaving tower (Btu/lb_m)
H	--	humidity
i_m	--	minimum rate of return
J	--	objective function value
K'	--	enthalpy transfer coefficient
K	--	overall heat transfer coefficient for the pond

(Continued)

L'	L'	length of tower (ft)
L/G	--	liquid over gas flow rates
PT	--	total pressure
OPCOST	--	operating cost of total cooling system
q	--	heat loss from pond
r	--	ratio of land cost to tower cost
RF	--	rate factor
t	--	temperature
t_{wb}	WBT	wet bulb temperature
t_o	--	base temperature
T_1	T1	temperature water entering tower
T_2	T2	temperature water leaving tower
T_e	--	equilibrium temperature
T_K	--	temperature in Kelvin
T_{PC}	--	water temperature leaving pond
T_{PH}	--	water temperature entering pond
TU	TU	tower units = $S_{t_1}^{t_2} \frac{dt}{(h'-h)}$
V'	V'	volume of tower (ft^3)
V_c	--	water velocity through condenser
V_S	--	water velocity in transportation system
W	W	water flow rate through tower (lb_m/hr)

GREEK SYMBOLS

$\alpha_{i,j}$	--	structural parameter, the stream goes to unit i, and leaves from unit j.
ℓ_v	--	heat of vaporization
ρ_w	RHO	density of water

CHAPTER 4

THE SYNTHESIS OF A CHEMICAL PLANT

INTRODUCTION

The synthesis of large, complex, heterogeneous systems has rarely been attempted. Fan et al. (1973) designed a wastewater treatment facility consisting of a trickling filter, an activated sludge reactor, and a secondary clarifier. Ichikawa and Fan (1973) and Osakada and Fan (1972) synthesized a two reactor, separator system. Siirola, et al. (1972) synthesized a chemical plant. Umeda, Hirai, and Ichikawa (1972) and Umeda, Shindo, and Tazaki (1972) synthesized a chemical process consisting of two CSTR reactors, two distillation columns, eight heat exchangers, and seven pumps.

The system synthesized by Umeda, Hirai, and Ichikawa (1972) was introduced by Bodman (1968). Originally the problem was to produce monochlorobenzene from benzene and chlorine. Dichlorobenzene was also produced in the reaction as an unfavorable by-product. In the course of their work, however, it was found that it was difficult to incorporate a scheme for removing the side product hydrochloric acid produced in the reaction. Therefore, a simplified reaction scheme replaced the original reaction scheme. Instead of producing monochlorobenzene from benzene and chlorine, component "B" was produced from "A". In addition component "B" could further react to produce an unfavorable by-product "C". Umeda, Hirai, and Ichikawa (1972) used a linear approximation with a signal flow, system reduction technique in their solution procedure. After the system was linearized, the signal flow, system reduction technique reduced the three recycle loops to only a single recycle loop. The accuracy of the numerical results of this approximation was sufficient for a preliminary design calculations.

In this thesis the system presented by Umeda, Hirai, and Ichikawa (1972) was resynthesized. A nonlinear formulation was used to simulate the process. Two optimal systems were synthesized, first by using a direct search with a structural parameter solution formulation and second, by using a direct search with an evolutionary structural parameter solution formulation.

DESIGN AND COST EQUATIONS

The design and cost equations are presented for each of the subsystems, the reactors, distillation columns, and heat exchangers. The combined system is then tentatively developed from the subsystems.

Reactor Equations

The reaction considered is

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C \tag{4.1}$$

where

B = desired product

$$K_1 = 3 \times 10^{14} e^{(-20/RgT)} \tag{4.2}$$

$$K_2 = 3 \times 10^{16} e^{(-25/RgT)} \tag{4.3}$$

Rg = gas constant

T = temperature in the reactor

Since constant flow stirred tank reactors are used, the conversions can be expressed as

$$X_A = 1 - \left(\frac{1}{1 + K_1\tau}\right) \tag{4.4}$$

$$X_B = 1 - \left(\frac{1}{1 + K_2\tau}\right) \tag{4.5}$$

where

X_i = conversion of the ith component

τ = residence time in the reactor

The mole fractions of the leaving materials in terms of the entering mole fractions and the conversions are

$$MF_{A,out} = MF_{A,in}(1 - X_A) \tag{4.6}$$

$$MF_{B,out} = (MF_{B,in} + MF_{A,in}X_A)(1 - X_B) \tag{4.7}$$

$$MF_{C,out} = (MF_{B,in} + MF_{A,in}X_A)(X_B) + MF_{C,in} \tag{4.8}$$

where

$M_{i,j}$ = mole fraction of the ith component (i = A,B,C,) and jth stream (j = in, out)

X_i = conversion of ith component

Distillation Column Equations

The distillation column can be thought of merely as a spilter as indicated in Fig. 4-1. Then only three flow rates and the compositions in these three streams need be considered for the mass balances. The ranking of the relative volatilities of the components must be considered in order to predict the separations. In this problem, the relative volatility of A is greater than that for B which is greater than that for C. The relative volatilities must be based on the relative volatility of the heavy key in the separation. The specification of the heavy key is, of course, then considered in the sequencing. For example, if component A is removed from the top of the distillation column, component A is the light key. Component B is the heavy key and the following equations can be derived, where the symbols are defined in Fig. 4-1.

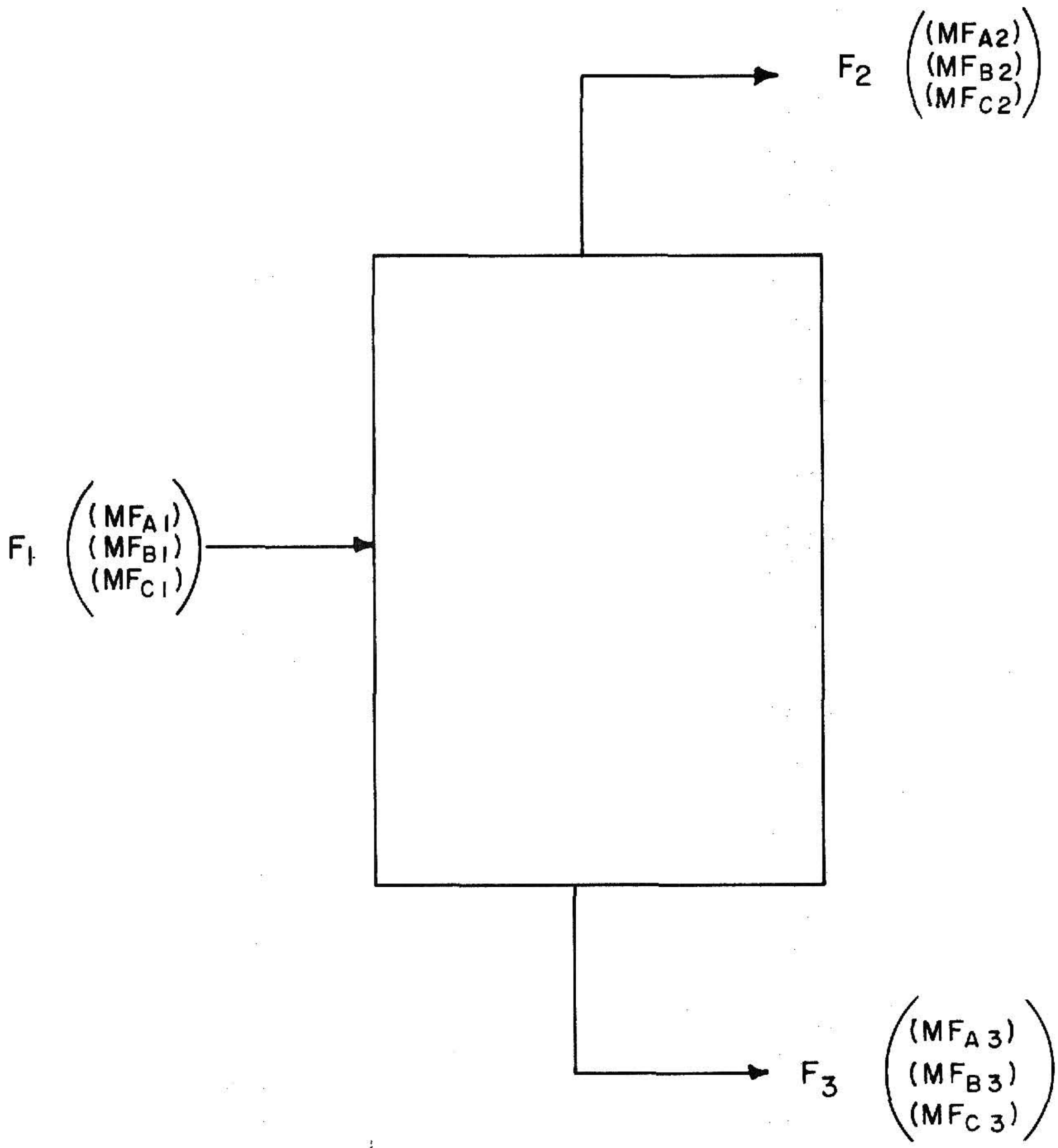


Fig. 4-1. Representation of a distillation column.

$$MF_{C,2} = 0$$

$$F_3 = S_L\ F_1\ MF_{A,1} + F_1\ MF_{B,1}\ S_H + F_1\ MF_{C,1}$$

$$F_2 = (1 - S_L)\ F_1\ MF_{A,1} + (1 - S_H)\ F_1\ MF_{B,1}$$

$$MF_{A,3} = (S_L\ F_1\ MF_{A,1})/F_3$$

$$MF_{A,2} = \frac{(1 - S_L)\ F_1\ MF_{A,1}}{F_2} \tag{4.9}$$

$$MF_{B,3} = \frac{S_H\ F_1\ MF_{B,1}}{F_3}$$

$$MF_{B,2} = \frac{(1 - S_H)\ F_1\ MF_{B,1}}{F_2}$$

$$MF_{C,3} = \frac{F_1\ MF_{C,1}}{F_3}$$

When component A and component B are removed from the top of the column, component C becomes the heavy key. This gives rise to the following equations.

$$MF_{A,3} = 0$$

$$F_3 = S_L\ MF_{B,1} + S_H\ F_L\ MF_{C,1}$$

$$F_2 = MF_{A,1}\ F_1 + (1 - S_L)\ F_1\ MF_{B,1} + (1 - S_H)\ F_1\ MF_{C,1}$$

$$MF_{B,3} = \frac{S_L\ F_1\ MF_{B,1}}{F_3} \tag{4.10}$$

$$MF_{C,3} = \frac{S_H\ F_1\ MF_{C,1}}{F_3}$$

$$MF_{A,2} = \frac{MF_{A,1}\ F_1}{F_3}$$

$$MF_{B,2} = \frac{(1 - S_L)\ F_1\ MF_{B,1}}{F_2}$$

$$MF_{C,2} = \frac{(1 - S_H)\ F_1\ MF_{C,1}}{F_2}$$

where

S_H = fraction of the heavy key in the bottoms of the column

S_L = fraction of the light key in the bottoms of the column.

Component B can be removed from either the top or bottom of the first column. If component B is taken from the top of the first column, component B will be removed from the bottom of the second column. Then equation (4.10) should be used on the first column and equation (4.9) should be used on the second column. If component B is taken from the bottom of the first column, component B will be removed from the top of the second column. Then equation (4.9) should be used on the first column and equation (4.10) should be used on the second column.

Finally, the reflux ratio needed to achieve the above separation can be calculated using the Underwood equation (Van Winkle, 1967).

$$R = (R/R_m)\ \left(\frac{MF_{A,2}\ \alpha_A}{\alpha_A - \theta} + \frac{MF_{B,2}\ \alpha_B}{\alpha_B - \theta} + \frac{\alpha_C\ MF_{C,2}}{\alpha_C - \theta}\right) \qquad (4.11)$$

where

R = reflux ratio or the liquid flow rate divided by the distillate flow rate

R_m = minimum reflux ratio

α_i = relative volatility of the ith component with respect to the heavy key, i = A, B, C, AV

θ = numerical value that satisifies the equation (Van Winkle, 1967)

$$0 = \frac{\alpha_A\ MF_{A,1}}{\alpha_A - \theta} + \frac{\alpha_B\ MF_{B,1}}{\alpha_B - \theta} + \frac{\alpha_C\ MF_{C,1}}{\alpha_C - \theta} = 1 - q \qquad (4.12)$$

The minimum number of trays in the column is calculated using a modification of Fenske's equation as used by Umeda, Hirai, and Ichikawa (1972).

$$N_m = \frac{\ln\left(\frac{(1 - S_{LL})(S_{HH})}{(S_{LL})\ (1-S_{HH})}\right)}{\ln\ (\alpha_{AV})} \tag{4.13}$$

where

N_m = minimum number of trays

$\alpha_{AV} = [(\alpha_{LK})(\alpha_{HK})]^{0.5}$

$S_{LL} = 1 - [\frac{F_2\ MF_2\ \text{Light Key}}{(F_1 MF_1\ \text{Light Key})}]$

$S_{HH} = 1 - [\frac{(F_2\ MF_2\ \text{Heavy Key})}{(F_1\ MF_1\ \text{Heavy Key})}]$

The actual number of trays is then computed from the Gilland correlation as used by Umeda, Hirai, and Ichikawa (1972).

$$N = \frac{N_m + e^{\phi}}{1 - e^{\phi}} \tag{4.14}$$

where

$\phi = 2.3\ \{0.9[\frac{(R-R_m)}{R+1}] - 0.17\}$

Finally, the diameter of the column is calculated as

$$D = \sqrt{\frac{4(\text{Vapor Flowrate})\ (T)\ (Rg)}{(3600)\ (\pi)}}$$

where

Rg = gas constant

T = absolute temperature in the column

Combined System

The combined system is then tentatively developed from the subsystems which contain the reactors, distillation columns, pumps, and heat exchangers.

Structural parameters, splitting fractions, are used at mixing points to determine the fraction of the flow of the original stream that is diverted. At mixing points, molar balances are performed to find the flow rates and compositions of the resulting stream.

Figure 4-2 illustrates the combined system before any optimization has been performed. The reactor subsystem is arranged so that if β_3 (the fraction of stream 2 that is diverted to stream 3) = 1.0 and if β_7 (the fraction of stream 4 that is diverted to stream 7) = 0.0, the system becomes a stirred-reactors-in-series system (Fig. 4-3). If β_3 = 0.5 and β_7 = 1.0, the system becomes two reactors in parallel system (Fig. 4-4).

The distillation subsystem is arranged so that the product, component B, can be removed from either the top or bottom of the second column. If component B is removed from the top of the second column, it must have been removed from the bottom of the first column (see Fig. 4-5). If component B is removed from the bottom of the second column, it must have been removed from the top of the first column. The distillation columns are connected so that either of the above two sequencing schemes can be achieved in the optimization procedure as indicated in Fig. 4-5.

Equipment Costs ($/Unit)

$$\text{Reactor cost} = 520 + 436\,[\tau(\text{Flowrate})]^{0.61} \qquad (4.14)$$

(Blecker, 1973)

Distillation cost = tray cost + tower cost

$$\text{tray cost} = 70\,\left(\frac{N}{0.5}\right)\left[D\left(\frac{10.8}{4.0}\right)\right]^{1.9} \qquad (4.15)$$

(Hendry and Hughes, 1972)

$$\text{tower cost} = (4.34)\ (2500)\ (D)\ (10.8\ \left[\frac{(N+1)(\text{tray space})\ 3.28}{40}\right] \qquad (4.16)$$

(Hendry and Hughes, 1972)

$$\text{Exchanger cost} = 726 + 566\ (\text{Area}/0.09)^{0.61} \qquad (4.17)$$

for fluid-fluid heat exchange (Blecker, 1973)

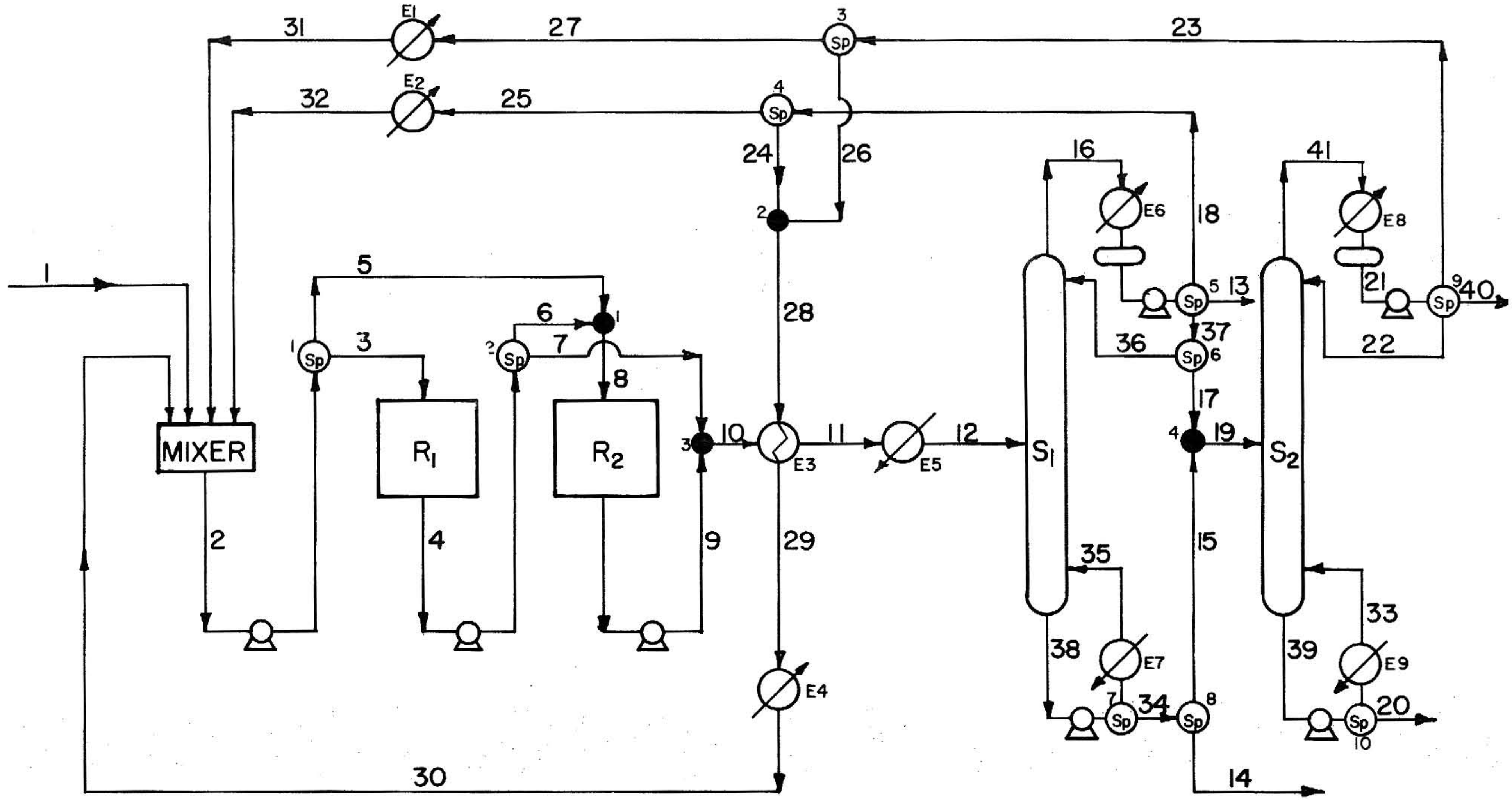


Fig.4-2. The combined system before optimization.

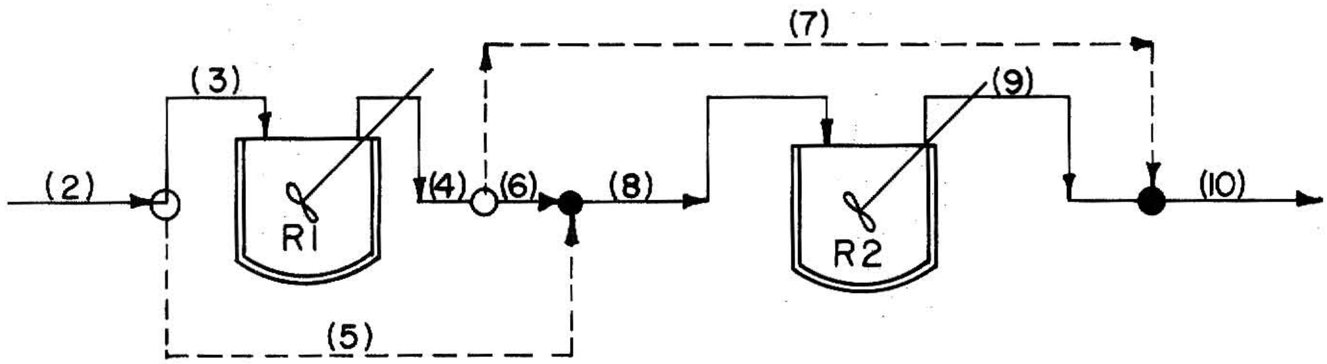


Fig. 4-3. Reactor system with series structure.

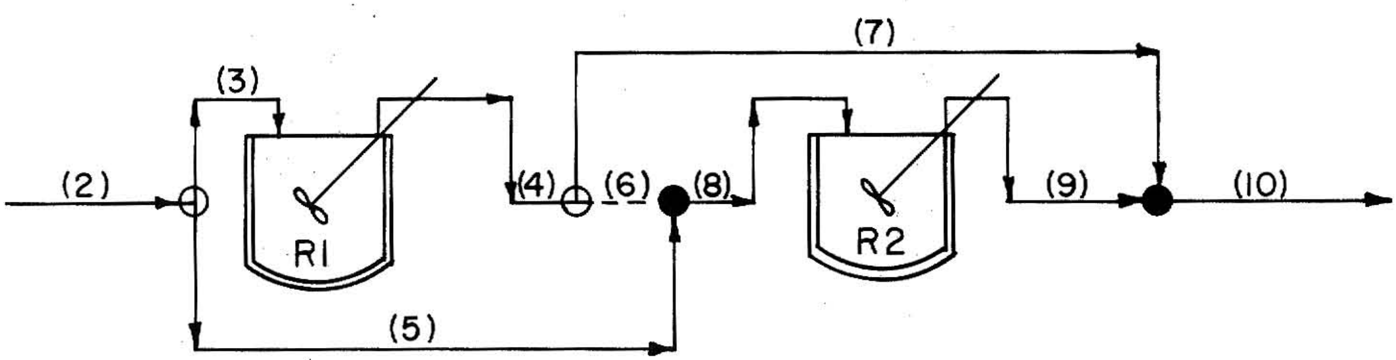
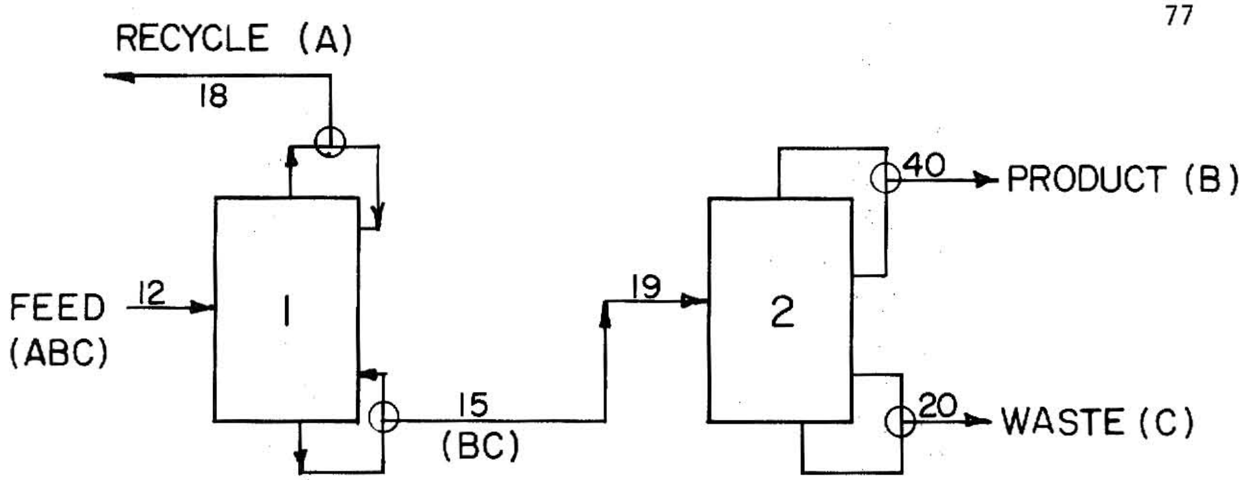


Fig. 4-4. Reactor system with parallel structure.



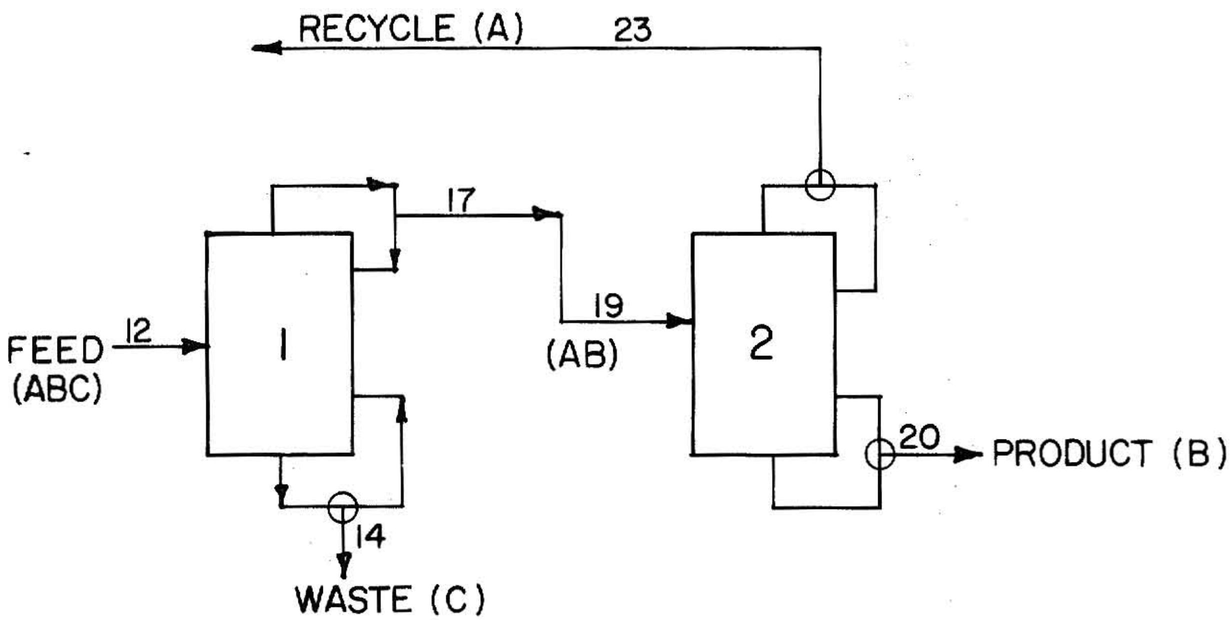


Fig. 4-5. Representation of the distillation sequencing schemes.

Exchanger cost for vapor-fluid heat exchanger (Blecker, 1973) $= 37290\ (\text{Area}\ (0.01076))^{0.65}$ (4.18)

pump cost $= 215\ (\text{Volumetric Flowrate})^{0.6}$ (Blecker, 1973) (4.19)

Operating costs

The operating costs consist of the cost of utility cold water and that of steam at \$0.017/ton and \$2.20/ton respectively. Cooling water is used both in the reactors and heat exchangers, but the steam is only used in the heat exchangers.

Objective Function

The objective function for the optimal synthesis of a chemical plant e.g. the system under consideration, can be the unaflow profit function, the rate of return profit function, the payout time profit function, or the venture profit function (Rudd and Watson, 1968). The choice as to which profit function to use is somewhat subjective. In this thesis, only the unaflow profit function has been used.

The unaflow profit function is dependent on the depreciation schedule used. Both a straight line and a sum of digits depreciation schedule can be used (Jelen, 1968). In this thesis only the straight line depreciation schedule is used.

The unaflow profit function is computed in five steps (Jelen, 1968). First the present worth of the total initial capital expense, IT, is computed. The second step is to compute the inflated total initial capital expense, CIX, to account for the inflation of the 1972 cost models presented in equations (4.14), (4.15), (4.16), (4.17), (4.18), and (4.19). In the third step, the present worth of the inflated total initial capital expense, CIX, and the possible tax advantage, Cost p, is calculated. The fourth step is to convert the present worth of the inflated total initial capital expense and possible tax advantage, Cost p, to a yearly equipment cost, R_{TSC} with straight line depreciation and R_{TSD} with sum of digits depreciation.

All of the four steps above have been used to derive equations (4.24) and (4.25). In this one equation the inflated initial capital expense is converted to the yearly equipment cost, R_{TSC} with straight line depreciation and R_{TSD} with sum of digits depreciation. Figure (4-6) illustrates the above steps.

Finally, in step five, the unaflow profit function, UNAFLOW, is calculated from the values of the yearly sales, yearly raw material cost, yearly operating cost, the appropriate tax rate, and the yearly equipment cost.

All of the other profit functions, the payout time, the rate of return, and the venture worth, can then be computed in sequence. The rate of return is computed as the unaflow, UNAFLOW, divided by the inflated initial capital expense, CIX. The payout time is the inflated initial capital expense, CIX, divided by the sales. The venture profit is found from the values of the annual sales, raw material costs, the yearly operating costs, the inflated initial capital expense and the minimum rate of return.

All of the derivations described above are developed in detail in the following paragraphs.

First, the total initial capital expense, IT, is computed as

$$IT = \sum_{i=1}^{M} (\text{unit cost})_i \qquad (4.20)$$

where

$(\text{Unit cost})_i$ = cost for each piece of equipment

M = total number of pieces of equipment

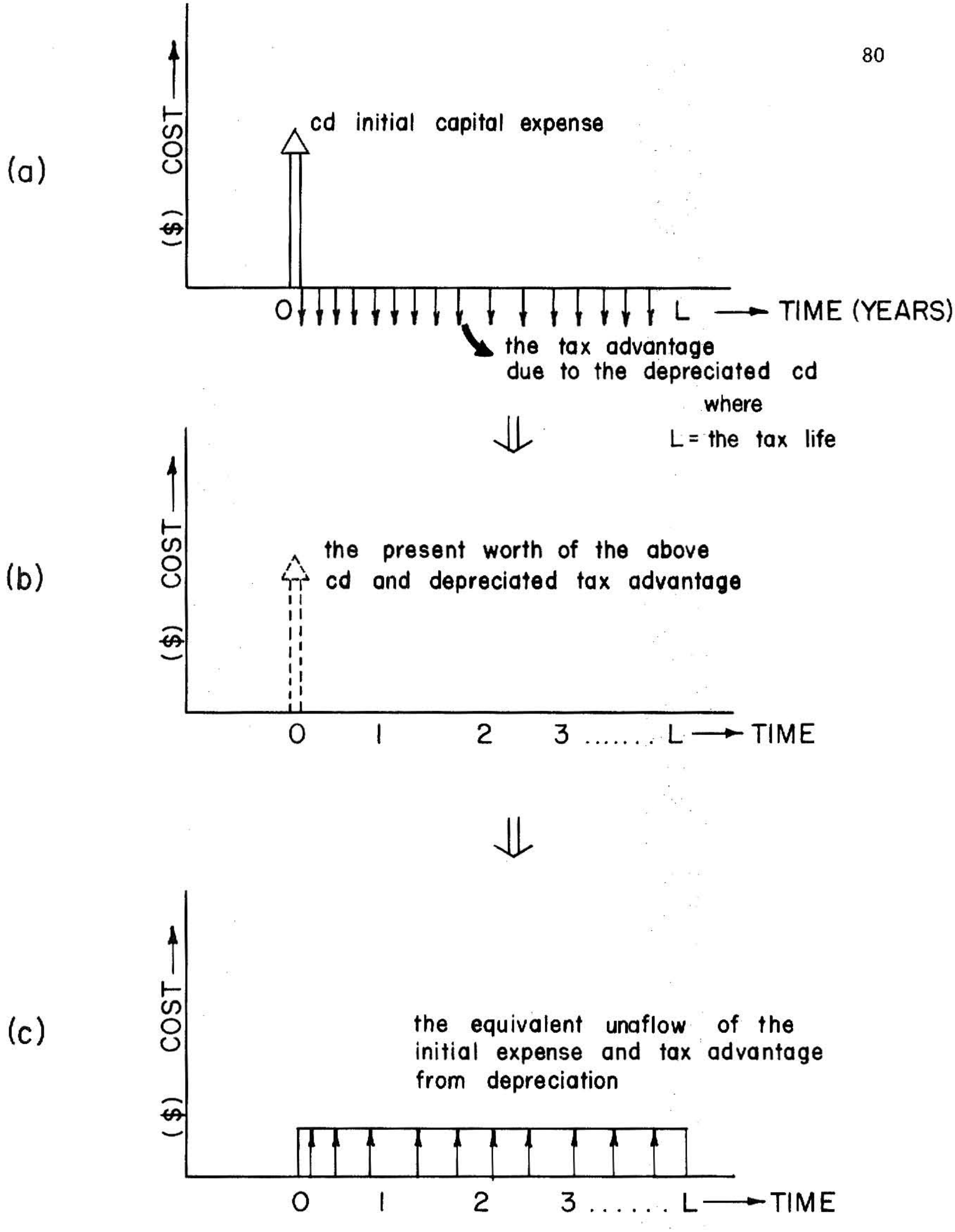


Fig. 4-6. Equivalent cost representations.

An inflated initial capital expense is then computed by using the Engineering News Record index (Blecker, 1973) and the Marshall Stevens index (Blecker, 1973) with a labor over material ratio of 0.6 (Blecker, 1973).

$$CIX = IT[(\frac{MSX}{330})(1 - 0.3) + 0.3\ (\frac{ENR}{1774})] \tag{4.21}$$

where

CIX = inflated initial capital expense

MSX = Marshall Stevens index

ENR = Engineering News Record index

Next the present worth of the cost of the inflated capital expense and possible tax advantage of the resulting depreciation is calculated as (Jelen, 1968)

$$Cost_{PSL} = (1 - t\ \Psi_{SL})(CIX) \quad \text{for straight line} \tag{4.22a}$$

$$Cost_{PSD} = (1 - t\ \Psi_{SD})(CIX) \quad \text{for sum of digits} \tag{4.22b}$$

where

$$\Psi_{SL} = \frac{1 - e^{-iL'}}{iL'} \quad \text{for straight line depreciation} \tag{4.23a}$$

$$\Psi_{SD} = \frac{2}{iL'}\ [1 - (\frac{1 - e^{-iL'}}{iL'}) \quad \text{for sum of digits depreciation} \tag{4.23b}$$

i = continuous interest

L' = tax life of equipment

Next the yearly equipment cost, R_{TSL} or R_{TSD}, is calculated for each type of depreciation.

$$R_{TSL} = (Cost_{PSL})[\frac{iL'}{L'(1-e^{-iL'})}] \quad \text{for straight line depreciation} \tag{4.24a}$$

$$R_{TSD} = (Cost_{PSD})[\frac{iL'}{L'(1-e^{-iL'})}] \quad \text{for sum of digits depreciation} \tag{4.24b}$$

By substituting equations (4.22a) and (4.23a) into equation (4.24a), and by substituting equations (4.22b) and (4.23b) into equation (4.24b) the following equations are derived.

$$R_{TSL} = \left(\frac{CIX}{L}\right)\left\{\left(\frac{iL}{1-e^{-iL}}\right)\right\} - t \quad \text{for straight line depreciation} \tag{4.25a}$$

$$R_{TSD} = \left(\frac{CIX}{L}\right)\left\{\left(\frac{iL}{1-e^{-iL}}\right) - \left(\frac{2t}{1-e^{-iL'}}\right) + \frac{2t}{iL}\right\} \tag{4.25b}$$

for sum of digits depreciation

The unaflow, UNAFLOW, can be computed from values of the sales of product, SALES; the cost of raw material, RM Cost; and the operating cost, Op Cost, as

$$\text{UNAFLOW} = (\text{SALES} - \text{RM Cost} - \text{Op Cost})(1 - t) - R_T \tag{4.26}$$

where

RM Cost = raw material cost

SALES = income from sales of product

Op Cost = operating cost

t = tax rate

$R_T = R_{TSL}$ or R_{TSD} depending on which depreciation scheme is used.

The rate of return is then defined as the unaflow per year divided by the initial investment.

$$\text{Rate of Return} = \frac{\text{Unaflow}}{\text{CIX}} \tag{4.27}$$

The pay out time as defined in "Capital and Operating Costs of Pollution Control Equipment Modules" (Blecker, 1973) is

$$\text{Pay Out Time} = \frac{\text{CIX}}{\text{SALES}} \tag{4.28}$$

and finally the venture profit can be computed as

$$\text{Venture Profit} = (\text{Sales} - \text{RM cost} - \text{operating costs})(1-t) - i_m \text{ CIX} \tag{4.29}$$

It should be noted that the usual types of profit functions considered in systems synthesis are very crude. In one study the following objective was considered.

$$\text{Profit} = (\text{Sales} - \text{RM Cost} - \text{OP Cost}) - \frac{\text{Investment}}{L} \qquad (4.30)$$

where

RM Cost = raw material cost

Op Cost = operating cost

Several researchers have used a venture profit (Hendry and Hughes, 1972; Umeda, Hirai, and Ichikawa, 1972; Rudd and Watson, 1968) which is

$$\text{Profit} = (\text{Sales} - \text{RM Cost} - \text{operating expenses}) - i_m(\text{investment})$$

However, i_m is a crude measure of the possible success of the process considered and only ball park figures are available for its estimation. The unaflow profit function, equation (4.26), proposed in this work is a much more rigorous consideration of the economic problem.

SOLUTION METHOD

Computational Procedure

The computational procedure starts by picking a set of independent variables listed in Table 4.1. Next pick a flow rate, F_{12}, and two, e.q. $MF_{A,12}$ and $MF_{B,12}$, of the three mole fractions, $MF_{A,12}$, $MF_{C,12}$, and $MF_{B,12}$, of the components of the stream entering the first column. The value of the independent variable ϕ' determines whether the molar flow rate of stream 15 or 17 will be set equal to zero. Calculate the flow rates and compositions leaving the first column by using equations (4.9), (4.10), (4.11), and (4.12), the independent variables $R/R_{m,1}$, $S_{1,H}$, $S_{1,L}$, β_{14}, and a molar balance about the distillation column. Calculate the flow rates and compositions leaving the second column by using equations (4.9), (4.10), (4.11), and (4.12), the independent variables $R/R_{m,2}$, $S_{2,H}$, $S_{2,L}$, β_{23}, and a molar balance about the second distillation column. The flow rates of streams 28, 25, and 27 are found from flow rates, F_{23} and F_{18}, and from the independent variables, β_{25} and β_{26}. The compositions of streams 28, 25, and 27 are found from molar balances about the mixing points. The flow rates and compositions of streams 31, 32, and 30 are equal to those of streams 27, 25, and 28 respectively. The flow rate and composition of stream 2 is found by using a molar balance about the mixer with the flow rate and composition of streams 1, 31, 32, and 30 known. The flow rates of streams 5, 3, 6, 7, 8, 9, 10, and 11 are found by using the independent variables β_3 and β_7, and by applying a mole balance about the mixing points. Equations (4.2), (4.3), (4.4), (4.5), (4.6), (4.7), and (4.8), and a molar balance about the mixing points are used to determine the compositions in streams 5, 3, 6, 7, 9, 9, 10, and 11.

When the compositions, $MF_{A,11}$, $MF_{B,11}$, and $MF_{C,11}$, and flow rate F_{11} of stream 11 are known set the flow rate, F_{12}, and composition $MF_{A,12}$, $MF_{B,12}$, and $MF_{C,12}$, equal to the flow rate, F_{11}, and compositions $MF_{A,11}$, $MF_{B,11}$, and $MF_{C,11}$, of stream 11 respectively. The above procedure is repeated until flow rate 11, F_{11}, matches within one percent of flow rate 12, F_{12}, mole fraction of A in stream 11, $MF_{A,11}$, matches the mole fraction of A in stream 12, $MF_{A,12}$, within one percent, and the mole fraction of B in stream 11, $MF_{B,11}$, matcnes the mole fraction of B in stream 12, $MF_{B,12}$, within one percent.

The temperatures of the streams are found first by assuming that the top and bottom temperatures of the distillation columns are the molar weighted averages of the boiling points of the pure components, and second by making heat balances over each of the mixing points.

Equipment costs are found from equations (4.14), (4.15), (4.16), (4.17), (4.18), and (4.19). Equations (4.20), (4.21), (4.22), (4.23), (4.24), (4.25), and (4.26) are used to find the objective function value, UNAFLOW. If the user desires to use the other profit functions, payout time, rate of return and venture profit as the objective function, he should substitute for equation (4.26) one of the following equations; equation (4.27) for rate of return, equation (4.28) for payout time, or equation (4.29) for venture profit.

Direct Search

A direct search can be applied to this problem in a very straightforward manner since the problem is formulated with structural parameters. The optimization routine used in this thesis is a sequential random search. Chen and Fan (1975) developed this very effective search routine. It is used in this thesis because of its applicability to optimization problems with many independent variables. Specifically, the unaflow profit function, equation (4.26), listed in the earlier section, is used as the objective function. Sales is based on the flow rate of the product stream. The product has a minimum concentration of component B of 95% and can be withdrawn from stream 20 or stream 40. The set of independent variables are specified in Table 4.1 along with the ranges over which they may vary.

Evolutionary Approach

The evolutionary approach attempts to maximize the objective function with respect to the independent variables listed in Table 4.1 with an iterative technique (Ichikawa and Fan, 1973). First, the tentatively proposed total system is optimized. The resulting optimal solution is examined in order to determine a possible change in the structure that can cause an increase in the objective function value. If a change in the structure can be found that will cause an increase in the objective function value, the new structure is accepted and the new system is optimized. This process of optimization and examination is repeated until

TABLE 4.1 The List of Independent Variables

NDEPENDENT VARIABLE	RANGE	DESCRIPTION
T_2	30 to 60°C	temperature of stream 2
T_4	30 to 60°C	temperature of stream 4
T_9	30 to 60°C	temperature of stream 9
T_{11}	30 to 60°C	temperature of stream 11
1	0.5 to 2.5 hr.	residence time of the 1st reaction
2	0.5 to 2.5 hr.	residence time of the 2nd reaction
$S_{1,L}$	0.0 to 0.1	fraction of the light key in the bottom of the first column
$S_{1,H}$	0.9 to 1.0	fraction of the heavy key in the bottom of the first column
$S_{2,L}$	0.0 to 0.1	fraction of the light key in the bottom of the second column
$S_{2,H}$	0.9 to 1.0	fraction of the heavy key in the bottom of the second column
$R/R_{m,1}$	1.1 to 5.0	ratio of the reflux to the minimum reflux for the first column
$R/R_{m,2}$	1.1 to 5.0	ratio of the reflux to the minimum reflux in the second column
β_3	0.0 to 1.0	fraction of stream 2 diverted to stream 3
β_7	0.0 to 1.0	fraction of stream 4 diverted to stream 7
β_{36}	0.0 to 1.0	fraction of the tops leaving the second column diverted to stream 18
β_{14}	0.0 to 1.0	fraction of stream 34 diverted to stream 14
β_{23}	0.0 to 1.0	fraction of the difference between stream 41 and stream 22 diverted to stream 23
β_{26}	0.0 to 1.0	fraction of stream 23 diverted to stream 26
β_{25}	0.0 to 1.0	fraction of stream 18 diverted to stream 25
ϕ'	0.0 to 1.0	column sequence parameter

no new changes that will cause the objective function to increase can be found.

How the structural changes can be found is based on engineering judgment. For example, in the chemical plant synthesis under consideration, the mole fraction of the product in the stream entering the second column appears to be close to the desired product mole fraction in the tentatively proposed total system. Therefore, the final column was dropped as a proposed structural change in the next iteration. The new system is optimized and an optimal solution is obtained.

RESULTS AND DISCUSSION

Direct Search

The results of the optimization of the direct search are shown in Tables 4.2, 4.3, 4.4, and 4.5, which are, respectively, the independent variable list, the Flow Matrix, the Data Matrix, and the Cost Matrix.

Figure 4.4 illustrates the first optimal structure from the direct search. Both reactors and both columns are present when the product is withdrawn from the last column. Streams 13, 14, 26, 27, and 31 approach zero. The reactor subsystem is an approximately parallel system, with the first reactor being the larger of the two reactors. The composition of the feed of the second column is very close to the desired composition so that some improvement might be expected at this point in the synthesis.

A reformulation is next attempted with the direct search by allowing any stream which has a composition greater than the minimum product composition to be considered as a product stream. With this formulation more than one stream can be considered as a product stream. This new problem is then optimized and the results appear in Tables 4.6, 4.7, 4.8, and

TABLE 4.2 Optimal Results of First Direct Search

INDEPENDENT VARIABLES	OPTIMAL VALUE
T_2	33.3241
T_4	30.7809
T_9	30.0216
T_{11}	51.0150
τ_1	0.5209
τ_2	0.6096
$S_{1,L}$	0.0244
$S_{1,H}$	0.9622
$S_{2,L}$	0.0041
$S_{2,H}$	0.9226
$R/R_{m,1}$	1.2037
$R/R_{m,2}$	2.1714
β_3	0.1744
β_7	0.5735
β_{36}	1.0
β_{14}	0.0352
β_{23}	0.00761
β_{26}	0.0108
β_{25}	0.0073
ϕ'	0.0658

TABLE 4.3 Optimal Results After First Direct Search

** FLOW MATRIX **

STREAM	FLOW RATE (GMOLES/HR)	%A	%B	%C	TEMP (DEGREE C)
1	55233.0	0.1000000E 01	0.0000000E 00	0.0000000E 00	20.00
2	129488.1	0.9809027E 00	0.1909255E-01	0.4360286E-05	33.32
3	22589.5	0.9809027E 00	0.1909255E-01	0.4360286E-05	33.32
5	106898.5	0.9809027E 00	0.1909255E-01	0.4360286E-05	33.32
6	9633.3	0.5994113E 00	0.3942103E 00	0.6347742E-02	30.78
7	12956.3	0.5994413E 00	0.3942103E 00	0.6347742E-02	30.78
10	129488.0	0.5669309E 00	0.4254057E 00	0.7662121E-02	30.10
11	129488.0	0.5669309E 00	0.4254057E 00	0.7662121E-02	50.96
12	129769.8	0.5669118E 00	0.4254250E 00	0.7663250E-02	102.90
13	0.1	0.9717818E 00	0.2821829E001	0.0000000E 00	81.56
14	1965.7	0.3216776E-01	0.9500474E 00	0.1778471E-01	131.08
15	53950.8	0.3216776E-01	0.9500474E 00	0.1778471E-01	131.08
17	0.0	0.9717818E 00	0.2821829E-01	0.0000000E 00	81.56
18	73853.2	0.9717818E 00	0.2821829E-01	0.0000000E 00	81.56
19	53950.8	0.3216776E-01	0.9500474E 00	0.1778471E-01	131.08
20	1094.4	0.0000000E 00	0.1911344E 00	0.8088657E 00	165.97
23	402.0	0.3283383E-01	0.9657618E 00	0.1404446E-02	130.35
28	73316.6	0.9717262E 00	0.2827396E-01	0.8337804E-07	81.57
40	52454.2	0.3283383E-01	0.9657618E 00	0.1404446E-02	130.35

TABLE 4.4 Optimal Results After First Direct Search

** DATA MATRIX **

UNIT NO.	1	2	3	4	5	6	7	8	9
MIN REFLUX	0.35	0.30							
REFLUX RATIO	0.42	0.64							
MIN TRAYS	8.61	11.12							
NUMBER TRAYS	23.62	20.53							
DIAMETERS	1.07	1.03							
HEAT EXCH LD	1238.59	676.38	91686.44	0.00	228246.50	775324.80	911469.80	753279.30	804097.80
EXCH DEL TEMP	52.68	35.51	20.63	17.73	97.07	56.56	42.92	105.35	8.03
EXCH AREA	0.12	0.10	22.22	0.00	7.84	45.69	70.78	23.83	333.89
EXCH UTIL FLW	6881.	3758.	0.	0.	19458.	4307361.	77704.	4184886.	63551.
PUMP FLOW RATE	11.54	2.12	10.99	16.21	9.35	8.53	8.75		

TABLE 4.5 Optimal Results After First Direct Search

** COST MATRIX **

	TOTAL COSTS
UTIL TOTAL ($/HR)	16.17
SALES ($/YEAR)	5320223.00
RM COST ($/YEAR)	4031520.00
INVESTMENT ($)	637063.00
PROFIT FUNC ($) =	515095.40
UNIFLOW ($) =	515095.40
RATE OF RETURN (%) =	80.85
PAY OUT TIME (YEARS) =	1.24
VENTURE PROFIT ($) =	417160.70

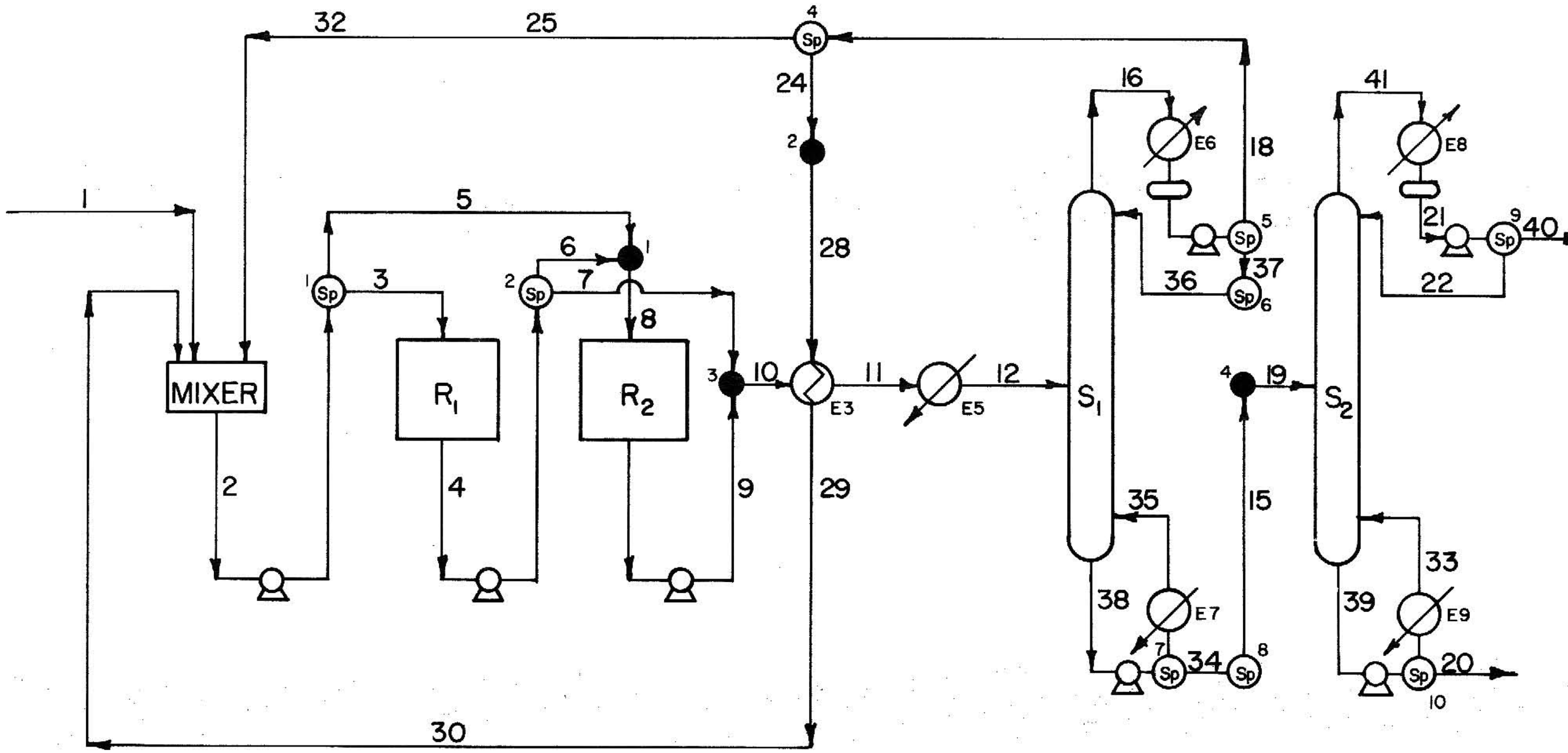


Fig.4-7. First optimal structure from the direct search.

TABLE 4.6 Optimal Results After Second Direct Search

INDEPENDENT VARIABLE	OPTIMAL VALUE
T_2	54.059
T_4	30.089
T_9	30.0001
T_{11}	30.8489
τ_1	0.5000
τ_2	0.9397
$S_{1,L}$	0.0357
$S_{1,H}$	0.9260
$S_{2,L}$	0.00267
$S_{2,H}$	0.9356
$R/R_{m,1}$	4.5900
$R/R_{m,2}$	1.4711
β_3	0.91053
β_7	0.86338
β_{36}	1.0
β_{14}	0.0
β_{23}	0.00033
β_{26}	0.85950
β_{25}	0.67548
ϕ'	0.02616

TABLE 4.7 Optimal Results After Second Direct Search

** FLOW MATRIX **

STREAM	FLOW RATE (GMOLES/HR)	%A	%B	%C	TEMP (DEGREE C)
1	55233.0	0.1000000E 01	0.0000000E 00	0.0000000E 00	20.00
2	130974.6	0.9682615E 00	0.3173784E-01	0.1740553E-06	54.06
3	119257.0	0.9682615E 00	0.3173784E-01	0.1740553E-06	54.06
5	11717.6	0.9682615E 00	0.3173784E-01	0.1740553E-06	54.06
6	16292.5	0.6181864E 00	0.3765221E 00	0.5290862E-02	30.09
7	102964.5	0.6181864E 00	0.3765221E 00	0.5290862E-02	30.09
10	130974.6	0.5655952E 00	0.4261899E 00	0.8214034E-02	30.07
11	130974.6	0.5655952E 00	0.4261899E 00	0.8214034E-02	30.83
12	131255.9	0.5655620E 00	0.4262227E 00	0.8215249E-02	102.99
13	0.1	0.9453293E 00	0.5467103E-01	0.0000000E 00	82.94
14	0.0	0.4770778E-01	0.9328743E 00	011941765E-01	130.34
15	55532.1	0.4770778E-01	0.9328743E 00	0.1941765E-01	130.34
17	0.0	0.9453293E 00	0.5467103E-01	0.0000000E 00	82.94
18	75723.8	0.9453293E 00	0.5467103E-01	0.0000000E 00	82.94
19	55532.1	0.4770777E-01	0.9328742E 00	0.1941764E-01	130.34
20	1147.1	0.0000000E 00	0.1204562E 00	0.8795438E 00	168.94
23	17.8	0.4871397E-01	0.9500087E 00	0.1277293E-02	129.53
28	24588.8	0.9447697E 00	0.5522959E-01	0.7968602E-06	82.97
40	54367.1	0.4871397E-01	0.9500087E 00	0.1277293E-02	129.53

TABLE 4.8 Optimal Results After Second Direct Search

** DATA MATRIX **

UNIT NO.	1	2	3	4	5	6	7	8	9
MIN REFLUX	0.26	0.29							
REFLUX RATIO	1.19	0.43							
MIN TRAYS	7.24	11.98							
NUMBER TRAYS	10.44	28.11							
DIAMETERS	1.35	0.98							
HEAT EXCH LD	4.54	6990.17	3385.94	0.00	320792.80	1235282.00	1441760.00	674496.40	725501.60
EXCH DEL TEMP	77.36	55.80	50.39	53.60	107.09	57.94	43.66	104.53	5.06
EXCH AREA	0.00	0.63	0.34	0.00	9.99	71.07	110.07	21.51	478.01
EXCH UTIL FLW	25.	38834.	0.	0.	27348.	6862679.	122912.	3747203.	61850.
PUMP FLOW RATE	11.69	11.16	2.71	22.31	14.88	7.64	7.84		

TABLE 4.9 Optimal Results After Second Direct Search

** COST MATRIX **

	TOTAL COSTS
UTIL TOTAL ($/HR)	18.99
SALES ($/YEAR)	5315063.00
RM COST ($/YEAR)	4031520.00
INVESTMENT($)	617946.00
PROFIT FUNC ($) =	502515.30
UNIFLOW ($) =	502515.30
RATE OF RETURN (%) =	81.32
PAY OUT TIME (YEARS) =	1.23
VENTURE PROFIT ($) =	407519.50

4.9, which are the variable list, the Flow Matrix, the Data Matrix, and the Cost Matrix. The obvious result is that streams 14 and 40 are both product streams. It can also be seen that heat exchangers 1, 2, and 4 are no longer needed in this design. Also in this design the second reactor is favored. Finally, both distillation columns are used as shown in Fig. 4-8. Their sizes are about the same.

Evolutionary Approach

Figure 4-2 is the tentatively proposed original structure of the combined two reactor, two distillation column system. The product is, at the beginning, only withdrawn from the top or bottom of the final column. The separation sequencing is performed by the optimization routine. Component A can be the light key in the first column and B can be the light key in the second column, or vice versa.

The product leaving the system will have a purity of at least 95% component B, and this will be sold at the price indicated in Table 4.10.

After the first optimization, the structure of the system is as illustrated in Fig. 4-7. Table 4.2 lists the values of the independent variables. Table 4.3 lists the Flow Matrix, consisting of all stream flow rates, compositions, and temperatures. Table 4.4 lists the Data Matrix, which consists of intermediate results such as column diameters and heat exchanger heat loads. Table 4.5 lists the Cost Matrix, which includes all of the unit costs, utility costs, profit function value, and alternative profit function values.

Next, according to the evolutionary design procedure, the system is examined to see if any changes can be made in the system's structure in order to increase the profit function. The composition of the stream entering the second column appears to be very close to the desired product

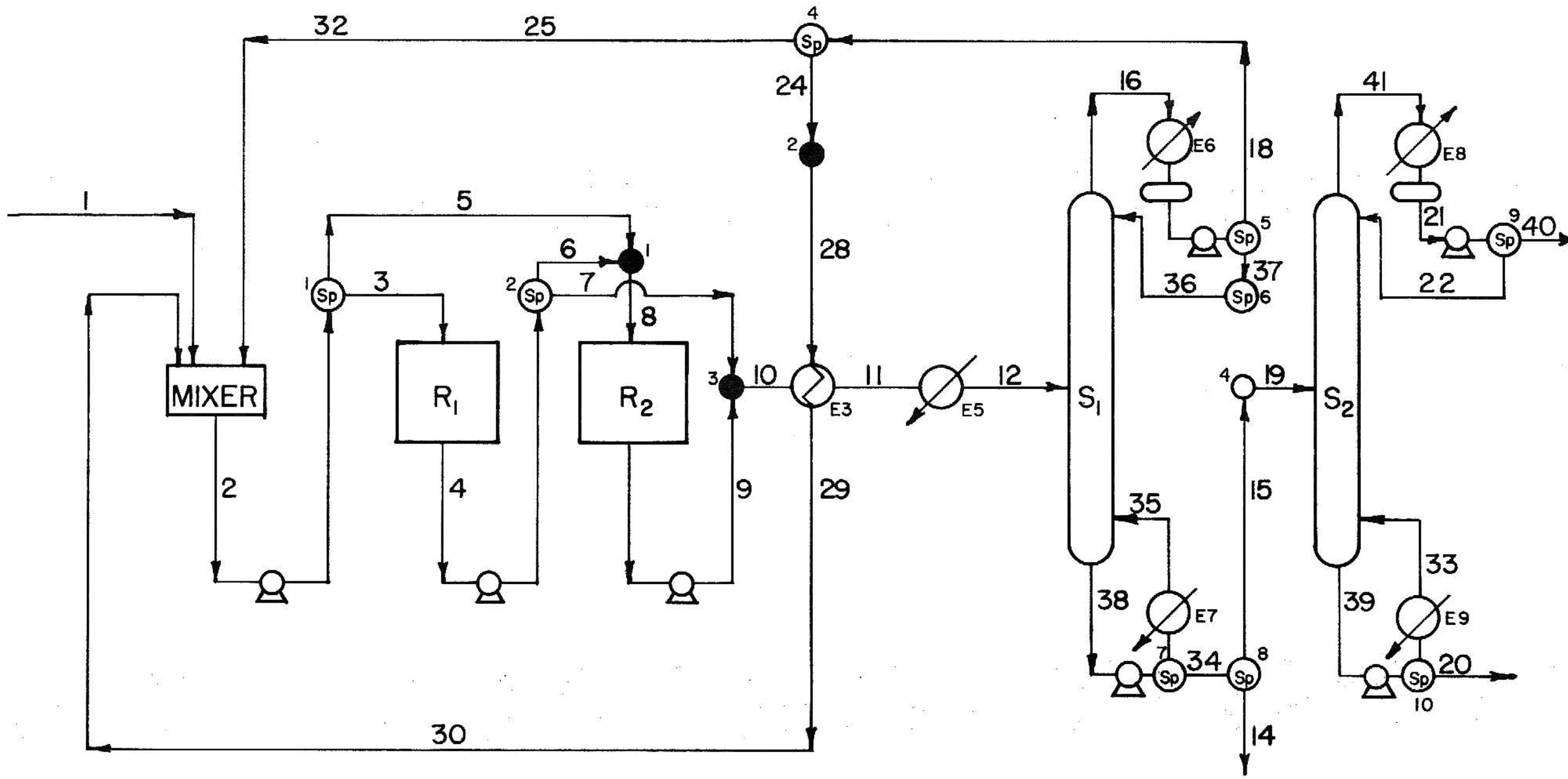


Fig. 4-8. Optimal structure from the second direct search.

TABLE 4.10 Design and Cost Data

Design basis		
Feed rate (ton/year)		40,000
Product specification (%)	min.	95.0
Specified data for equipment design		
Frequency factors	A_1	3.0×10^{14}
(1/hr)	A_2	3.0×10^{16}
Activation energy	E_1	20.0
(kcal/mole)	E_2	25.0
Heat of reaction	$-\Delta H_1$	60.0
(kcal/mole)	$-\Delta H_2$	30.0
Overall heat transfer coefficients	(for coolers)	200.0
(kcal/m^2hrC)	(for reboilers & condensers)	300.0
Tray spacing for towers (mm)		500.0
Tray efficiency (%)		50.0
Economic data		
Feed cost (cent/kg)		11.1
Product sales (cent/kg)		14.9
Utility costs		
cooling water (cent/ton)		1.7
steam ($/ton)		2.2
electric power (cent/kwh)		1.4
refrigeration (cent/10^6 kcal)		20.8
Minimum acceptable rate of return (%)		25.0
Tax (%)		50.0

(Umeda, Hirai, and Ichikawa, 1972)

composition of 95% of component B. A possible change would then be to remove the second column and increase the number of trays in the first column so that the product purity is achieved. In order to remove the second column, a new structure, in Fig. 4-8 is used with this structure. The product is removed from stream 13 or stream 14.

After the optimization, the structure of the new system is shown in Fig. 4-9. Tables 4.11, 4.12, 4.13, and 4.14, list the independent variables, Flow Matrix, Data Matrix, and Cost Matrix. The obvious difference between this final result and the earlier structure is that both the second column and one of the reactors have disappeared. Since the system is much simpler and the product purity is achieved, the resulting costs are lower as would be expected. The sales have had only a small change since the amount of product produced is unchanged.

The usual evolutionary design is accomplished by beginning with a simple system and then complicating the system to achieve the optimal design. The example presented here is the basic method in reverse. A complicated system has been simplified to achieve the optimal design. The basic idea of using an iterative technique of structuring and optimizing is unchanged.

The possibility of using any of the other systems synthesis techniques is discussed in the following paragraphs.

Dynamic Programming

Dynamic programming has not been used on this problem. One reason is that three state variables exist in the composition and flow rate problem, and temperature is added in the heat exchanger problem. One of the most limiting aspects of dynamic programming is the curse of dimensionality (Aris, 1964). The addition of each state variable increases the size of the problem by one order of magnitude. This problem has three state variables so that its solution with dynamic programming would take excessive

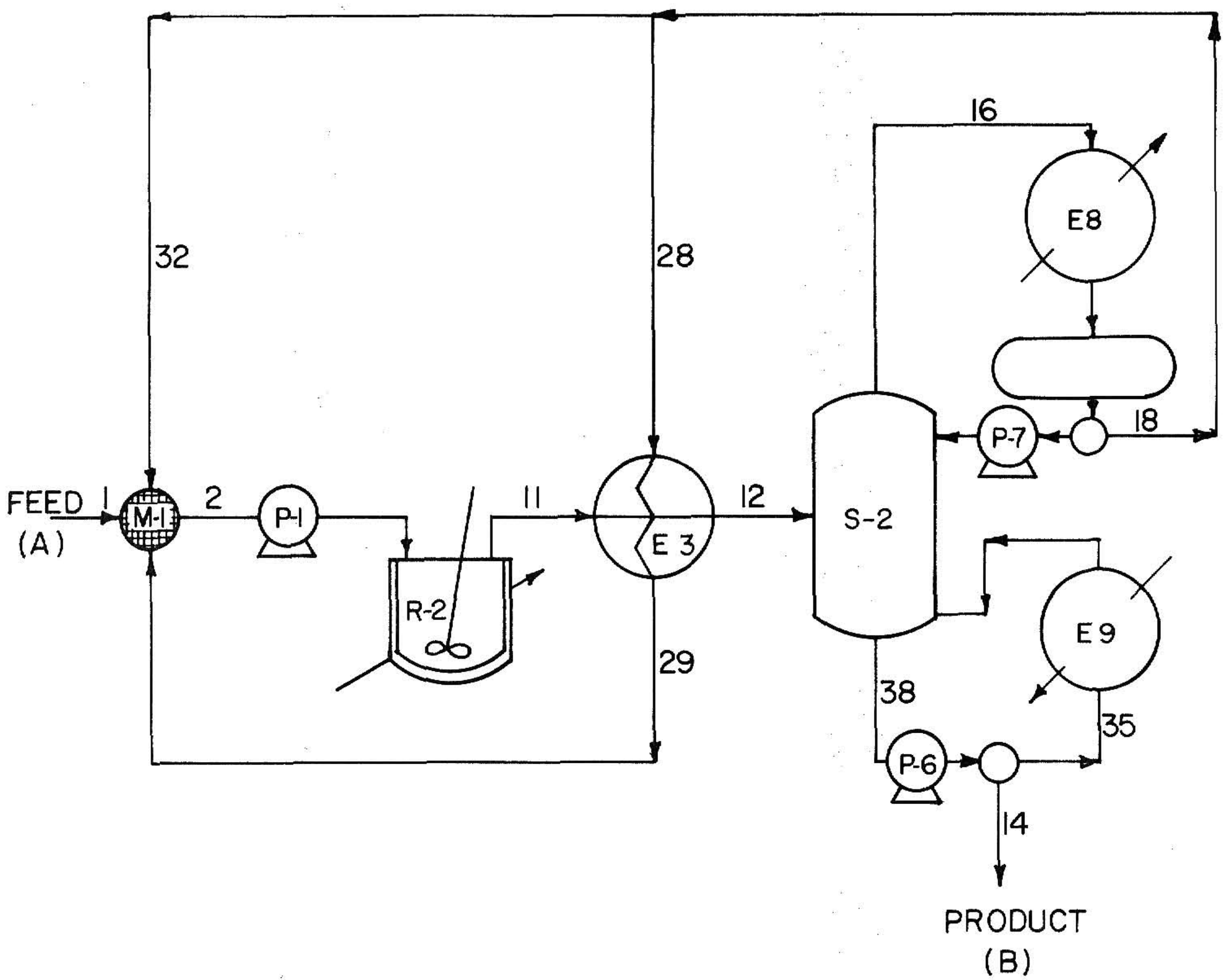


Fig. 4-9. Optimal structure of the evolutionary direct search.

TABLE 4.11 Optimal Results of Final Evolutionary Direct Search

INDEPENDENT VARIABLES	OPTIMAL VALUE
T_2	37.501
T_4	30.235
T_9	30.1715
T_{11}	37.3690
τ_1	1.5483
τ_2	1.1976
$S_{1,L}$	0.0072
$S_{1,H}$	0.9350
$S_{2,L}$	0.0323
$S_{2,H}$	0.9325
$R/R_{m,1}$	1.4492
$R/R_{m,2}$	3.7856
α_3	0.0000
α_7	0.1972
α_{36}	1.0
α_{14}	0.9989
α_{23}	0.90512
α_{26}	0.5320
α_{25}	0.3201
ϕ'	0.1761

TABLE 4.12 Final Results of Evolutionary Direct Search

** FLOW MATRIX **

STREAM	FLOW RATE (GMOLES/HR)	%A	%B	%C	TEMP (DEGREE C)
1	55233.0	0.1000000E 01	0.0000000E 00	0.0000000E 00	20.00
2	98915.2	0.9626618E 00	0.3733686E-01	0.1252495E-05	37.51
3	6.4	0.9626618E 00	0.3733686E-01	0.1252495E-05	37.51
5	98908.8	0.9626618E 00	0.3733686E-01	0.1252495E-05	37.51
6	5.1	0.3460544E 00	0.6361495E 00	0.2779588E-01	30.23
7	1.3	0.3460544E 00	0.6261495E 00	0.2779588E-01	30.23
10	98915.1	0.4063920E 00	0.5740638E 00	0.1954309E-01	30.17
11	98915.1	0.4063920E 00	0.5740638E 00	0.1954309E-01	37.32
12	99122.0	0.4063434E 00	0.5741112E 00	0.1954544E-01	111.73
13	0.3	0.9164773E 00	0.8352274E-01	0.0000000E 00	84.43
14	55431.5	0.4207911E-02	0.9598773E 00	0.3491467E-01	133.20
15	58.1	0.5207911E-02	0.9598773E 00	0.3491467E-01	133.20
17	0.0	0.9164773E 00	0.8352274E-01	0.0000000E 00	84.43
18	43633.0	0.9164773E 00	0.8352274E-01	0.0000000E 00	84.43
19	58.1	0.5208068E-02	0.95987735 00	0.3491467E-01	133.20
20	3.7	0.0000000E 00	0.4876168E 00	0.5123831E 00	153.52
23	49.2	0.5561456E-02	0.9919224E 00	0.2516374E-02	131.82
28	29693.9	0.9156728E 00	0.8432490E-01	0.2222206E-05	84.48
40	5.2	0.5561456E-02	0.9919224E 00	0.2516374E-02	131.82

TABLE 4.13 Final Results of Evolutionary Direct Search

** DATA MATRIX **

UNIT NO.	1	2	3	4	5	6	7	8	9
U R FLW	1348.	18763100.							
MIN REFLUX	0.39	0.28							
REFLUX RATIO	0.56	1.06							
MIN TRAYS	9.46	8.40							
NUMBER TRAYS	21.57	12.60							
DIAMETERS	0.87	0.04							
HEAT EXCH LD	59.66	11436.42	24363.19	0.00	-253614.10	510147.60	596953.20	976.56	1015.65
EXCH DEL TEMP	65.78	46.54	37.51	38.21	99.47	59.43	40.80	106.82	20.48
EXCH AREA	0.00	1.33	3.25	0.00	8.50	28.61	48.77	0.03	0.17
EXCH UTIL FLW	331.	63536.	0.	0.	21621.	2834154.	50891.	5425.	87.
PUMP FLOW RATE	8.84	0.00	9.51	12.51	6.14	0.01	0.01		

TABLE 4.14 Final Results of Evolutionary Direct Search

** COST MATRIX **

	TOTAL COSTS
UTIL TOTAL ($/HR)	10.46
SALES ($/YEAR)	5419120.00
RM COST ($/YEAR)	4031520.00
INVESTMENT ($)	313954.10
PROFIT FUNC($) -	619648.10
UNIFLOW ($) -	619648.10
RATE OF RETURN (%) =	197.37
PAY OUT TIME (YEARS) =	0.51
VENTURE PROFIT ($) =	571384.50

computer storage space and time. The second reason why dynamic programming has not been used in this problem is that several recycle loops exist. A solution procedure can be derived using dynamic programming but a large number of iteration steps is needed for the solution. Finally, this study is directed toward the understanding of methods of systems synthesis applied to problems of industrial size and complexity. Most industrial systems have more than three state variables and numerous recycle loops. Dynamic programming is not well suited for these systems, except in special applications.

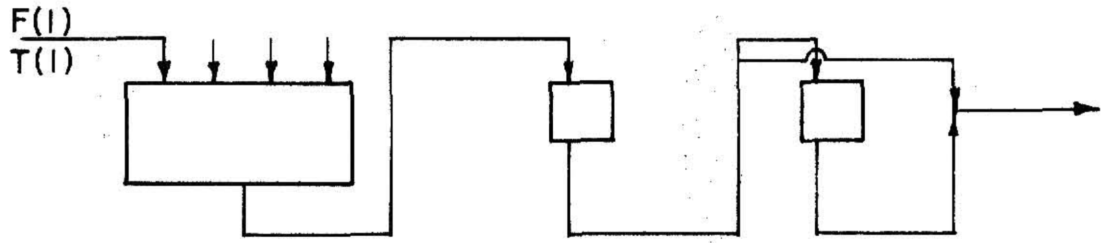
Heuristic Technique

The heuristic technique as presented by Siirola, Powers, and Rudd (1971) could be applied to the two reactor, two distillation problem, except that the heuristics needed for this problem are, first, not readily available and secondly, the accuracy of the individual heuristics cannot be evaluated. Of course, if some of the heuristics used cause the problem to approach the optimum then those heuristics can be said to be valid and accurate. But since the information received by the heuristic technique cannot be applied directly to different problems, then the selection of the heuristics is all important. If the proper heuristics are not chosen at the time of the problem formulation, then the solution will not be optimal.

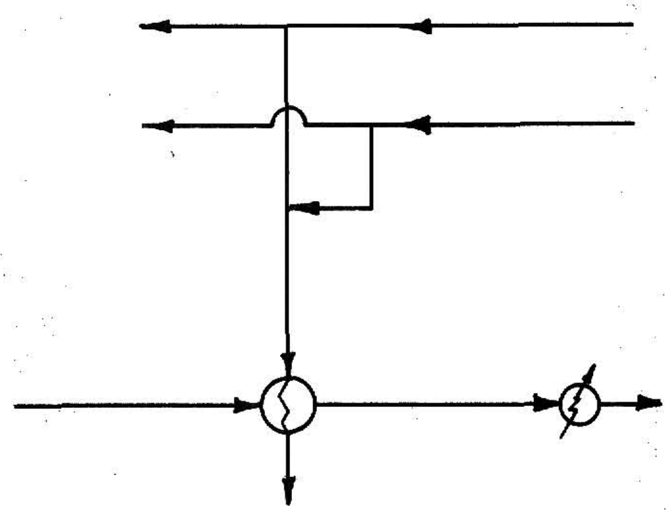
Decomposition

A decomposition method might be used to synthesize the chemical plant example. Figure 4-2 shows the combined system. Fig. 4-10 shows how the problem could be decomposed according to the decomposition approach of Osakada and Fan (1972) or the Lagrangian decomposition approach of Umeda (1972).

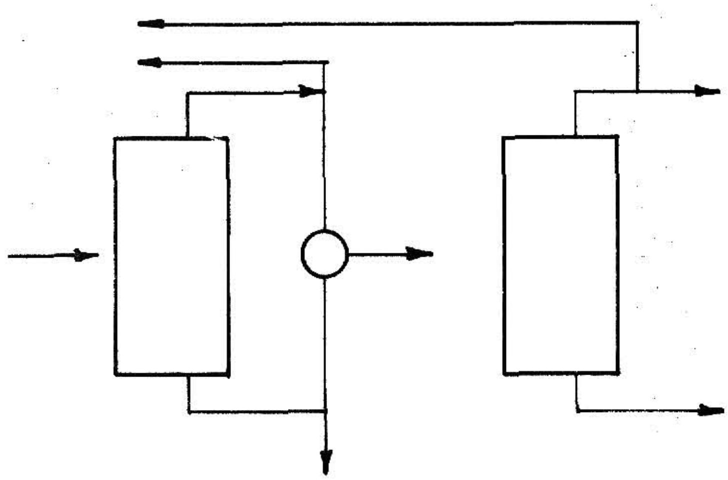
The combined system consisted of a direct search with twenty variables. The decomposition problem consists of four problems. The first level has a ten variable problem, a three variable problem, and a seven variable problem. The top level is a twenty-one variable, recombination problem.



The Reactor Sub-system



The Heat Exchange Sub-system



The Distillation Sub-system

Fig. 4-10. Decomposed chemical plant.

As indicated in the earlier section on decomposition approaches in systems synthesis, the space needed in the computer may be less for this problem, but the solution may require more time for the optimization than the original, nondecomposed problem.

Umeda, Shindo and Tasaki's (1972) feasible decomposition approach cannot be applied to this specific design problem because the number of coordination variables is larger than the number of internal independent variables. In fact, when Umeda, Shindo, and Tasaki (1972) attempted to solve this two reactor, two distillation column problem with the feasible decomposition method, they were arbitrarily forced to reduce the complexity of the systems structure. They assumed several of the streams of the original problem were zero before the optimization was attempted.

Other Techniques

Umeda and Ichikawa (1972) solved this problem with a linearizing technique. They were able to reduce the system by using a signal flow representation. The most dangerous problems with this technique are that the product stream and the number of units are specified at the time of linearization and internal results cannot be easily determined.

All of the linear techniques have been disregarded because the purpose of this work is to compare several systems synthesis techniques on large nonlinear systems. Both the branch and bound method and the feasible matrix, decision tree method have been used in energy integration and heat exchanger systems. Since the energy costs in this problem are relatively small, the inclusion of a separate energy optimization routine would not be justified. The theorem proving algorithm (Mahalce, 1974) cannot be used for optimal systems synthesis since the linkage of an economic package has not been accomplished. In addition, the problem of how to control the generation of designs to maximize the profit has not been solved.

CONCLUSION

The results of this work indicate that a direct search with the structural parameter solution formulation can be applied most effectively to the optimal synthesis of chemical processes, heterogeneous, nonlinear systems, similar to the example presented in this thesis.

An evolutionary structural parameter solution formulation is also used effectively on the optimal synthesis of a chemical process. The results of this work indicate that the evolutionary structural parameter solution formulation is less restrictive than the structural parameter solution formulation with respect to the types of structures that can be developed into optimal systems.

In addition no other systems synthesis techniques have been found that can be applied to this chemical plant example problem without using excessive computer time and computer storage space.

NOMENCLATURE

TEXT NOTATION	COMPUTER NOTATION	EXPLANATION
CIX	CIX	inflated capital expense
$Cost_p$		present worth of CIX plus tax advantage from depreciation
$Cost_{\bar{R}}$		unaflow of $Cost_p$
D	D_i	diameter of distillation column i=1, 2
ENR	ENR	Engineering News and Record index
F_k	F(K)	gram molar flow rate in stream k
i	CONI	continuous interest per year
i_m	0.25	minimum annual return
IT	IT	sum of unit costs
K_i	K_{ij}	kinetic parameter of ith reaction, jth reactor
L	11	tax life of equipment
$MF_{i,j}$	MF(i,K)	mole fraction of component i; j=in for mole fractions entering the reactor, j=out for mole fractions, k=stream leaving the reactor
$MF_{i,k}$	MF(i,K)	mole fraction of component i, i=A, B, C in stream k, k=1, 2, . . ., 41
MSX	MSX	Marshall Stevens index
N	Ni	number of trays in distillation column, i=1, 2
N_m	NMi	minimum number of i=1, 2 trays in distillation column

(continued)

OPERAT COST		operating cost per year
	P	profit function
q	1.0	parameter in Underwood equation
R	Ri	reflux ratio i=1, 2
R_g	R	gas constant
R_i	RTAX	yearly equipment cost with straight line depreciation i=TSL, or sum of digits depreciation i=TSD
R_m	RMi	minimum reflux ratio in distillation column i=1, 2
RM_{cost}	RMCOST	raw material cost
R/R_{mi}	RRMi	ratio of reflux over minimum reflux for the ith column i=1, 2
t	TAXRAT	tax rate
T		temperature
T_k	T(K)	temperature of kth stream
S_H		fraction of heavy key in bottoms of distillation column i-1, 2
$S_{i,H}$	SiH	fraction of heavy key in bottoms of ith column i=1, 2
$S_{i,L}$	SiL	fraction of light key in bottoms of ith column i=1, 2
S_L		fraction of light key in bottoms of column
SALES	SALES	yearly income from product sales
UNAFLOW	UNAFLW	a unaflow yearly profit
X_i	Xij	conversion of ith component, i=A, B; j=1, 2

Greek Symbols

α_i	REVOLj	relative volatility of component i, i=A, B, C, AV with respect to the heavy key, j=1, 2, 3

(continued)

β_m	ALPHM	structural parameter m=3, 7, 36, 14, 23, 26, or 25
θ	JA	parameter in Underwood equation
π	3.14159	3.14159
τ_i	TAUi	residence time in ith reactor
ϕ	JA2	parameter in Gilland correlation
ϕ'	PICK	column sequence parameter
Ψi		parameter based on type of depreciation; i=SL for straight line, i=SD for sum of digits

Chapter 5

CONCLUSIONS AND RECOMMENDATIONS

The choice of the most promising systems synthesis technique for homogeneous systems depends on the type of system to be synthesized. Heat exchanger networks can be most efficiently solved with the feasible matrix decision tree approach. Separation sequencing can be solved most efficiently with the dynamic programming list processing technique. Multicomponent reactor networks can be synthesized effectively by using a direct search with a structural parameter solution formulation.

Nonlinear, nonserial, heterogeneous systems have been most effectively synthesized by the heuristic technique and by direct search with an evolutionary structural parameter solution formulation. The heuristic technique relies on the choice of a set or sets of heuristic rules and the method of selection of a heuristic rule from a set. The advantages of the heuristic technique is that the desired accuracy and the time needed to solve the problem can be adjusted by varying the generality of the heuristics used.

The synthesis of nonlinear, nonserial, heterogeneous systems in this paper has been done with a direct search with an evolutionary structural parameter solution formulation. The problem of heuristic rule selection of the heuristic technique is now replaced with the problems of unit selection and stream existence. Engineering judgement is used to derive the initial system structure, and to alter the basic structure in the evolutionary manner.

When the two reactor, two distillation column problem was synthesized with only a direct search with the structural parameter solution formulation, the choice of the product stream of the initial system structure forced the derived optimal solution to be only a local optimum. A direct solution of the problem was attempted by allowing any of the streams leaving the system to become a product stream if the concentration of the desired product in the respective streams was greater than the minimum product requirement. This search also found a local optimum. Finally the direct search with the evolutionary structural parameter solution formulation was attempted and the result appears to be the global optimum.

Since both the heuristic technique and the direct search with an evolutionary structural parameter solution formulation depend, to a great extent, on engineering judgement, the possibility of developing new optimal systems different from the present concept of design is very remote. The development of a design is dependent on the designer's concept of the problem and the boundary of the development is the designer's imagination. Both the heuristic technique and the direct search with the evolutionary structural parameter solution formulation depend on the designer's concept of the problem.

The only technique used in systems synthesis that approaches the design of totally new, previously unconceived designs is the theorem proving algorithm. A synthesis technique that was an extension to the theorem proving algorithm that could not only economically evaluate possible designs but also force convergence to optimal designs would have a very high probability of being able to generate new concepts in design.

One of the basic problems associated with the theorem proving technique is the computer language in which the basic program is written, LISP 1.5. Whether the problem can be effectively solved with another computer language, which can be used for computations, Fortran, should be first determined. If the translation becomes a major problem, then the linkage between programs written with different compilers must be set up.

Secondly, a thermodynamic package must be available with program controlled access. In order to generate new designs, all types of information, in addition to that anticipated by the designer, must be supplied to the systems synthesizer.

Finally, the problem of how to control the development of designs to force convergence to optimal designs must be solved. Since the development of the designs may be performed in the computer language LISP 1.5 and the economic evaluation of the design will probably be done in Fortran, the linkage of the programs written with different compilers is again a problem. In addition, the theory of optimization as used in systems synthesis will have to be modified to force the development of optimal designs. Since the development of a design occurs in the evaluation portion of the theorem proving algorithm, the condition portion, these conditions must be altered in some manner to derive optimal solutions. How optimization theory will do this is not obvious.

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APPENDIX A

Computer Formulation for Cooling System Design

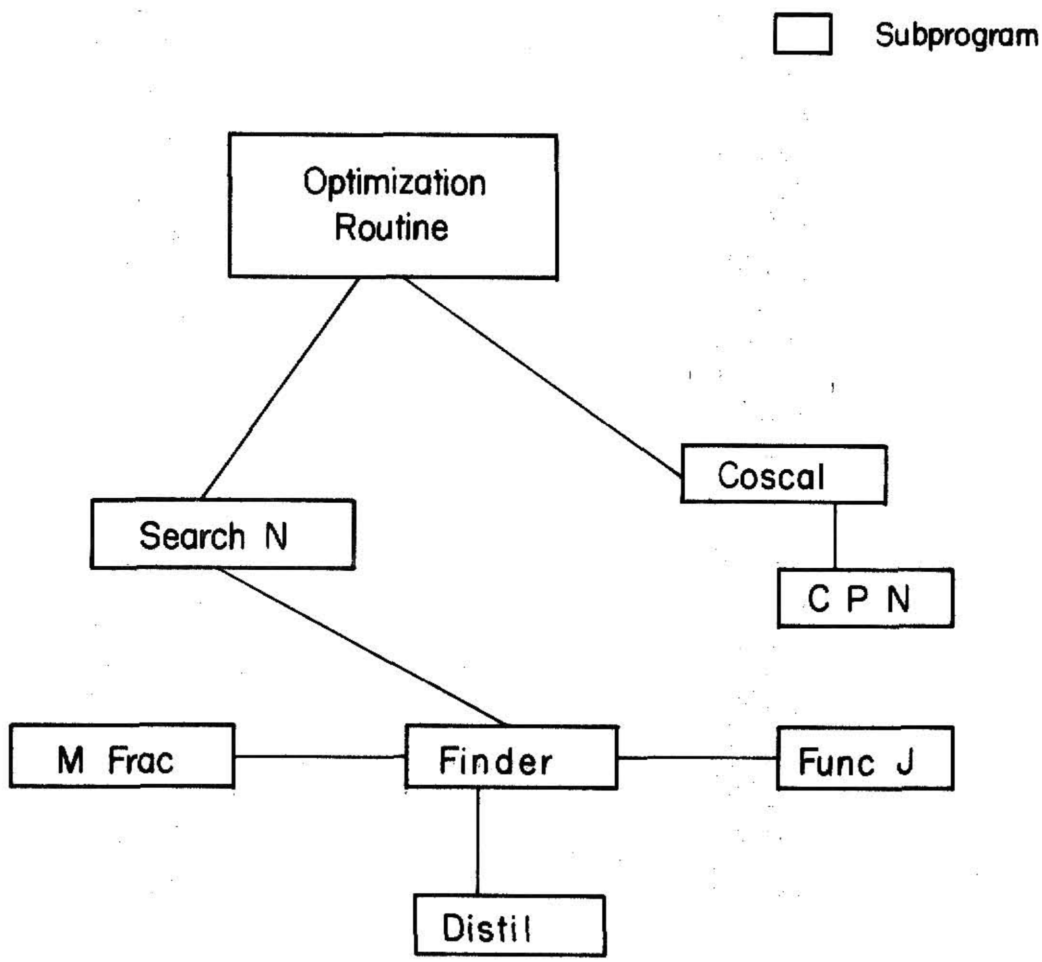
```
      STOP
  315 WRITE  (6, 325)  IT
  325 FORMAT (///, 20X,'INT. AND EXT. POINTS MERGE AT ITERATION NO.',
     1          I3, /////// )
      STOP
      END
C
      SUBROUTINE PROBE (JOB, MESG)
      DIMENSION  BOD(360), B(360)
      DIMENSION  XB(50,2)
      DIMENSION  X(50), G(50), MAC(50), NV(50), S(50), XHI(50), XLO(50)
      COMMON/COMON/ T1,T2,TWB
      COMMON /COMON1/ A2,B2,C2,D2
      COMMON/ONE/ X1,X2,X3,X4,X5,X6,X7,X8,X9,X10,X11,X12,X13,X14,X15,X1
     1   ,X17,X18,X19,X20,X21,X22,X23,X24,X25,X26,X27,X28,X29,X30,X31,
     2   X32,X33,X34,X35,X36,X37,X38,X39,X40,X41,X42,X43,X44,X45,X46,
     3   X47,X48,X49,X50
      COMMON /TWO/ G, MAC, NA, T, GSQ, F, FP, IX, NC, ND, NS, NSS, NV
      COMMON/THREE/ S, PEN, XHI, XLO,XB
      EQUIVALENCE  (X1, X(1))
      GO TO  (901,902,903 ),  JOB
  901 MESG = 1
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
      DO 150 I=1,ND
      XHI(I) = 1.
      XLO(I) = 0.
  150 CONTINUE
      XLO(11)=82.D0
      XHI(11)=115.D0
      XLO(15)=81.D0
      XHI(15)=115.D0
      DOLKWH=0.010D0
      A2=70.434690D0
      B2=-7362.698D0
      C2=0.006952100
      D2=-9.D0
      TC=95.D0
      TH=115.D0
      X15=TC
      CPRHO=8.3D0
      Q=163.7D6/60.D0/24.D0*30.D0*CPRHO
      DOLTU=5.07D0
      TE=80.D0
      TWB=75.D0
      PKMIN=150.D0/60.D0/24.D0
      APFT2=4250.D0/43560.D0
      T2=TH
       DOLPP=0.0
      RETURN
  902 MESG = 1
      X10=1.0D0
      X3 =1.0D0
      X1 = X9*X10
      A31=1.D0-X1
      X2=A31
      A21=X(1)
      A31=X(2)
      X11=TC
      A11=0.0D0
      A12=X(3)
```

```
      TC=X(11)
      TTC=X(15)
      RNG=TH-TTC
      T1=TTC
      A11=1.0D0-A31-A21
      A32=1.D0-A12
      TPC=(TC-A11*TH-A12*A21*TTC)/(A31+A32*A21)
      RF=HINTGL(T1,T2,RNG)
      GPM=Q/((TH-TC)*CPRHO)
      GPM=163.7D6/60.D0/24.D0
      DOLTCW=DOLTU*GPM*RF*A21
      TPH=(TH*A31+TTC*A32*A21)/(A31+A32*A21)
      XXX=(TPH-TE)/(TPC-TE)
      IF  ( XXX. LT. 1.)  GO TO 200
      GO TO 300
  200 MESG = 2
      RETURN
  300 CONTINUE
      DOLPD=CPRHO*GPM*ALOG((TPC-TE)/(TPH-TE))*(A21*A32+A31)*(-APET2)/(
     CPKMIN)
10    F=DOLPP+DOLPD+DOLTCW
      TOP=0.011* GPM*RF*0.746D0*DOLKWH*8400.D0*A21
      VELS=GPM/(60.D0*7.48D0*3.14D0*10.D0)
      RE=2.D0*VELS*62.4D0/0.00067200
      FFAC=0.04D00/RE **0.16D0
      STRA=2.D0*FFAC*VELS**2.D0*2000.D0      /(32.17D0*2.D0)
      VELC=GPM*(24.D0)**2/(60.D0*7.48D0*3.14D0*4500.D0)
      RE=     VELC*62.4DC/(.00067200*12.D0)
      FFAC=0.04D00/RE **0.16D0
      COND=2.D0*FFAC*VELC**2*12.D0*12.D0/(32.17D0*2.D0)
      FTOT=STRA+COND+30.D0
      PHP=FTOT*GPM*62.4D0/(0.4D0*60.D0*7.48D0*550.D0)
      POP=PHP*0.746D0*DOLKWH*8400.D0
      F=POP+TOP+0.0937D0*(DOLTCW+DOLPD)
C THE CONSTRAINTS ARE NOW CALCULATED
      G(1)=10.D0-VELS
      G(2)=10.D0-VELC
      X4 = RF
      X5 = TPH
      X6=DOLPP
      X7 = DOLPD
      X8 = DOLTOW
      X12=TPC
      X13=TH
      X14=GPM
      X15=TTC
      X16=VELS
      X17=VELC
      X18=POP
      X19=TOP
      X20=FTOT
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
      IX = 1
      FP = F
      GSC = 0
      PEN = 0.
      IF  (NA .EQ. 0)  RETURN
      DO 910  II = 1, NA
      I = MAC(II)
      IF  (G(I) .GE. 0.)  GO TO 910
```

```
      NV(I) = NV(I) + 1
      GSQ = GSQ + G(I)**2
      PEN = PEN + S(I)*G(I)
  910 CONTINUE
      IF  (GSQ .EQ. 0 )  RETURN
      IX = 2
      FP = F + T*GSQ - PEN
      RETURN
  903 MESG = 1
      RETURN
      END
C
       SUBROUTINE RANDOM (IX, IY, RM)
      IY = IX*65539
      IF (IY) 10, 20, 20
   10 IY = IY + 2147483647 + 1
   20 RM = IY
       RM = RM* .4656613E -9
      RETURN
      END
      FUNCTION HINTGL(T1,T2,RNG)
      HINTGL=RNG*(Y(T1+0.100*RNG)+Y(T1+.400*RNG)+Y(T2-.400*RNG)+Y(T2-.1(
     CO*RNG))/4.D0
      RETURN
      END
      FUNCTION Y(T)
      COMMON/COMON/ T1,T2,TWB
      CVERG=0.6D0
      H1=HS(TWB)
      ZIP= CVERG*(T2-T1)
      HL=H1+ZIP *((T-T1)/(T2-T1))
      Y=1.D0/(HS(T    )-HL)
      RETURN
      END
      FUNCTION HS(TF)
      COMMON /COMON1/ A2,B2,C2,D2
      TK=((TF-32.D0)/1.8D0)+273.1D0
      P2ATM= EXP(A2+B2/TK+C2*TK+D2*ALOG(TK))
      HS=0.240D0*TF+(18.D0*P2ATM/(29.D0*(1.D0-P2ATM)))*(1061.D0+0.444D0*
     CTF)
      RETURN
      END
$ENTRY
$STOP
```

APPENDIX B

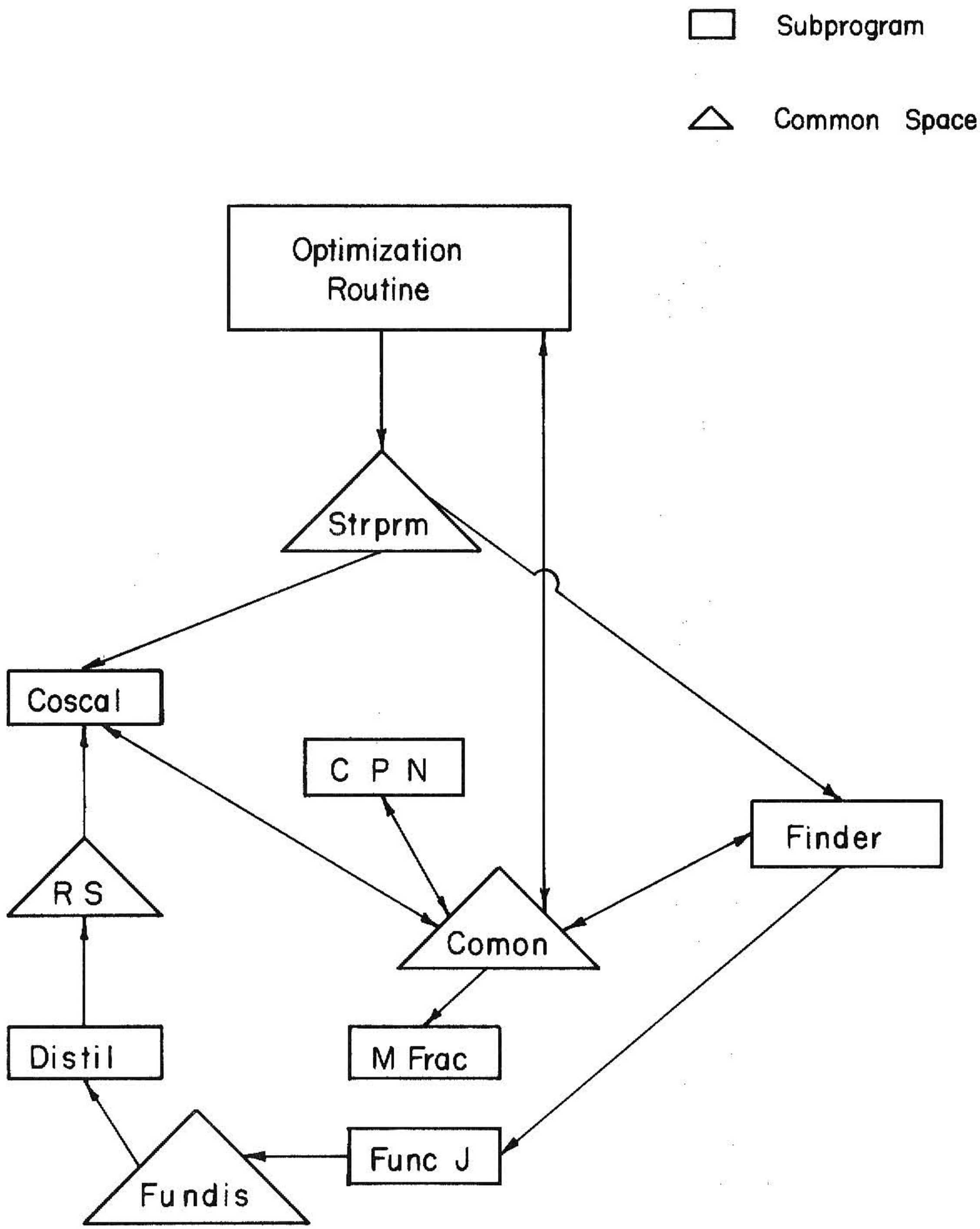
Subroutine Argument Map for Chemical Plant Design



The argument map for the chemical plant design.

APPENDIX C

Subroutine Common Space Map for Chemical Plant Design



The common space map for the chemical plant design.

APPENDIX D

Computer Formulation for the Chemical Plant Design

```
  270 CONTINUE
      FB(2) = FB(3) + T*FB(4)-BPEN
  290 FB(6) = BIG
  300 CONTINUE
  100 CONTINUE
      CALL PROBE (3, MESG)
       WRITE (6, 310)
  310 FORMAT  (////, 20X, 'JOB ACCOMPLISHED.', ////  )
      STOP
  315 WRITE  (6, 325) , IT
  325 FORMAT (///, 20X,'INT. AND EXT. POINTS MERGE AT ITERATION NO.',
     1          I3, /////// )
      STOP
      END
C
      SUBROUTINE PROBE (JOB, MESG)
      REAL HIGH(3),LOW(3),XX(3),MF(3,41),T(41),F(41),MSX
      INTEGER DEPRCI,PROFUN
      DIMENSION  BOD(360), B(360)                                         P.0
      DIMENSION  XB(50,2)
      DIMENSION  X(50), G(50), MAC(50), NV(50), S(50), XHI(50), XLO(50)
      COMMON/ONE/ X1,X2,X3,X4,X5,X6,X7,X8,X9,X10,X11,X12,X13,X14,X15,X16
     1   ,X17,X18,X19,X20,X21,X22,X23,X24,X25,X26,X27,X28,X29,X30,X31,
     2    X32,X33,X34,X35,X36,X37,X38,X39,X40,X41,X42,X43,X44,X45,X46,
     3    X47,X48,X49,X50
      COMMON /TWO/ G, MAC, NA,TT, GSQ,FF, FP, IX, NC, ND, NS, NSS, NV
      COMMON/THREE/ S, PEN, XHI, XLC,XB
      COMMON/DAT/ MSX,ENRX,DEPRCI,PROFUN,CONI,TAXRAT
      CCMMON/CCMON/F,MF,T
      COMMON/STRPRM/ALPH3,ALPH7,ALPH36,ALPH14,ALPH23,ALPH25,ALPH26,T2,T4
     C,T9,T11,TAU1,TAU2,S1L,S1H,S2L,S2H,RRM1,RRM2,PICK,CT11
      EQUIVALENCE  (X1, X(1))
      GO TO  (901,902,903 ),  JOB
  901 MESG = 1
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
      MSX=330.0
      ENRX=1774.0
      DEPRCI=2
      PROFUN=1
      CONI=0.1
      TAXRAT=0.5
      HIGH(1)=500000
      HIGH(2)=1.0
      HIGH(3)=1.0
      LOW(1)=55233
      LOW(2)=0.0
      LOW(3)=0.0
      F(1)=55233.
      MF(1,1)=1
      MF(2,1) =0
      MF(3,1)=0
      CALL CCSCAL(PFUNC,JOB)
      RETURN
  902 MESG = 1
      XX(1)=552330.
      XX(2)=0.3333
      XX(3)=0.3339
33    ALPH3=X1
      ALPH7=X2
      ALPH36=X3
```

```
      ALPH14=X4
      ALPH23=X5
      ALPH25=X6
      ALPH26=X7
      T(2)=X8
      T(4)=X9
      T(9)=X10
      CT11=X11
      TAU1=X12
      TAU2= X13
      S1L=X14
      S1H=X15
      S2L=X16
      S2H=X17
      RRM1=X18
      RRM2=X19
      PICK=X20
      CALL SERCHN(XX,MESG)
      IF(MESG.EQ.2) RETURN
      CALL CCSCAL(FF,JOB)
      FF=-FF
      X21=T(11)
      X22=F(12)
      X23=MF(1,12)
      X24=MF(2,12)
      X25=MF(2,2)
      G(1)=T(27)-T(31)
      G(2)=T(25)-T(32)
      G(3)=T(11)-T(10)
      G(4)=AMAX1(MF(2,13),MF(2,14),MF(2,20),MF(2,40))-0.95
      G(5)=F(33)-100.
      G(6)=F(35)-100.
      G(7)=T(12)-T(11)
C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
      IX = 1
      FP = FF
      GSQ = 0
      PEN = C.
      IF  (NA .EQ. 0)  RETURN
      DO 910  II = 1, NA
      I = MAC(II)
      IF  (G(I) .GE. 0.)  GO TO 910
      NV(I) = NV(I) + 1
      GSQ = GSQ + G(I)**2
      PEN = PEN + S(I)*G(I)
  910 CONTINUE
      IF  (GSQ .EQ. 0 )  RETURN
      IX = 2
      FP = FF+TT*GSQ - PEN
      RETURN
  903 MESG = 1
      DO 32 I=1,25
       X(I)=XB(I,1)
32    CONTINUE
      XX(1)=XB(22,1)
      XX(2)=XB(23,1)
      XX(3)=XB(24,1)
      GO TO 33
      RETURN
      END
```

```
C
      SUBROUTINE RANDOM (IX, IY, RM)
      IY = IX*65539
      IF (IY) 10, 20, 20
   10 IY = IY + 2147483647 + 1
   20 RM = IY
      RM = RM* .4656613E -9
      RETURN
      END
C      ****************************************************************
      SUBROUTINE SERCHN(X,MESG)
      REAL X(3),HIGH(3),LOW(3),FOUND(3)
      COMMON/NOGOOD/BADSOL
      DO 10 I=1,25,1
      CALL FINDER(X,FOUND)
      X(1)=FOUND(1)
      X(2)=FOUND(2)
      X(3)=FOUND(3)
      CALL FINDER(X,FOUND)
      IF(ABS(X(1)-FOUND(1)) .LT.500. ) GO TO 11
      X(1)=FOUND(1)
      X(2)=FOUND(2)
      X(3)=FOUND(3)
10    CONTINUE
      MESG=2
11    CONTINUE
1     RETURN
      END
C      ****************************************************************
      FUNCTION    CP(N)
      COMMON/COMON/F,MF,T
      REAL  CP,F(41),MF(3,41),T(41),CPA,CPB,CPC
      CPA=0.0325
      CPB=0.03585
      CPC=0.0342
      CPN=MF(1,N)*CPA+MF(2,N)*CPB+MF(3,N)*CPC
      CP=CPN
      RETURN
      END
C      ****************************************************************
      SUBROUTINE MFRAC(N,M)
      REAL F(41),MF(3,41),T(41)
      COMMON/COMON/F,MF,T
      MF(1,N)=MF(1,M)
      MF(2,N)=MF(2,M)
      MF(3,N)=MF(3,M)
      RETURN
      END
C      ****************************************************************
      SUBROUTINE FINDER(X,FOUND)
      REAL X(3),FOUND(3),NF12,NMFA12,NMFB12,F(41),MF(3,41),T(41),JA,K11
     C,K12,K22,K21
      INTEGER N,W
      COMMON/COMON/F,MF,T
      COMMON/STRPRM/ALPH3,ALPH7,ALPH36,ALPH14,ALPH23,ALPH25,ALPH26,T2,T4
     C,T9,T11,TAU1,TAU2,S1L,S1H,S2L,S2H,RRM1,RRM2,PICK,CT11
      COMMON/NOGOOD/BADSOL
      COMMON/XXX/K11,K12,K21,K22,XA1,XA2,XB1,XB2
      R=0.001987
      F(12)=X(1)
```

```
      MF(1,12)=X(2)
      MF(2,12)=X(3)
      MF(3,12)=1-X(2)-X(3)
      REVOLA=21.0
      REVOLB=4.2
      REVOLC=1.0
      COLUMN=1
      IF(PICK.LT.0.5          ) GO TO 100
      W=2
      JA=FUNCJ(2,12)
      CALL DISTIL(W     ,F(12),MF(1,12),MF(2,12),MF(3,12),S1H,S1L,REVOL1,
     CREVOL2,REVOL3,RRM1,F2,F3,F(36),F(16),F(38),F(35),MF(1,16),MF(2,16
     C),MF(3,16),MF(1,38),MF(2,38),MF(3,38),JA,COLUMN)
      F(15)=0.000001
      ALPH13=ALPH14
      ALPH14=0.99999
      F(18)=ALPH36*(F(16)-F(36))
      F(13)=(F(16)-F(36)-F(18))*ALPH13
      F(17)=F(16)-F(36)-F(18)-F(13)
100   IF(PICK.GE.0.5          ) GO TO 200
      W=1
      JA=FUNCJ(1,12)
      CALL DISTIL(W     ,F(12),MF(1,12),MF(2,12),MF(3,12),S1H,S1L,REVOL1,
     CREVOL2,REVOL3,RRM1,F2,F3,F(36),F(16),F(38),F(35),MF(1,16),MF(2,16
     C),MF(3,16),MF(1,38),MF(2,38),MF(3,38),JA,COLUMN)
      F(17)=0.00001
      F(18)=ALPH36*(F(16)-F(36))
      F(13)=F(16)-F(36)-F(18)
200   CALL MFRAC(36,16)
      CALL MFRAC(35,38)
      CALL MFRAC(18,16)
      CALL MFRAC(37,16)
      CALL MFRAC(13,16)
      F(37)=F(16)-F(18)
      F(34)=F(38)-F(35)
      F(14)=F(34)*ALPH14
      F(15)=F(34)-F(14)
      F(19)=F(15)+F(17)
      CALL MFRAC(17,16)
      CALL MFRAC(15,38)
      MF(1,19)=(F(15)*MF(1,15)+F(17)*MF(1,17))/F(19)
      MF(2,19)=(F(15)*MF(2,15)+F(17)*MF(2,17))/F(19)
      MF(3,19)=(F(15)*MF(3,15)+F(17)*MF(3,17))/F(19)
      COLUMN=2
      IF(PICK.LT.0.5          ) GO TO 300
      JA=FUNCJ(1,19)
      W=1
      CALL DISTIL(W,F(19),MF(1,19),MF(2,19),MF(3,19),S2H,S2L,REVOL1,REVO
     CL2,REVOL3,RRM2,F2,F3,F(22),F(41),F(39),F(33),MF(1,41),MF(2,41),MF(
     C3,41),MF(1,39),MF(2,39),MF(3,39),JA,COLUMN)
      IF(F(41).LT.0.0) F(41)=1.0
      IF(F(33).LT.0.0) F(33)=0.00001
300   IF(PICK.GE.0.5) GO TO 400
      W=2
      JA=FUNCJ(2,19)
      CALL DISTIL(W,F(19),MF(1,19),MF(2,19),MF(3,19),S2H,S2L,REVOL1,REVO
     CL2,REVOL3,RRM2,F2,F3,F(22),F(41),F(39),F(33),MF(1,41),MF(2,41),MF(
     C3,41),MF(1,39),MF(2,39),MF(3,39),JA,COLUMN)
      IF(F(41).LT.0.0) F(41)=1.0
      IF(F(33).LT.0.0) F(33)=1.0
```

```
400   F(23)=(F(41)-F(22))*ALPH23
      CALL MFRAC(23,41)
      F(21)=F(41)
      CALL MFRAC(21,41)
      F(20)=F(39)-F(33)
      CALL MFRAC(20,39)
      N1=20
      M1=39
      CALL MFRAC(N1,M1)
      F(26)=F(23)*ALPH26
      F(27)=F(23)-F(26)
      F(25)=F(18)*ALPH25
      F(24)=F(18)-F(25)
      F(28)=F(26)+F(24)
      F(29)=F(28)
      F(30)=F(29)
       F(31)=F(27)
      F(32)=F(25)
      CALL MFRAC(33,39)
      CALL MFRAC(22,41)
      CALL MFRAC(40,41)
      F(40)=F(41)-F(23)-F(22)
      CALL MFRAC(26,41)
      CALL MFRAC(24,16)
      MF(1,28)=(F(26)*MF(1,26)+F(24)*MF(1,24))/F(28)
      MF(2,28)=(F(26)*MF(2,26)+F(24)*MF(2,24))/F(28)
      MF(3,28)= (F(26)*MF(3,26)+F(24)*MF(3,24))/F(28)
      CALL MFRAC(30,28)
      CALL MFRAC(25,18)
      CALL MFRAC(29,28)
      CALL MFRAC(31,23)
      CALL MFRAC(27,23)
      CALL MFRAC(32,18)
      F(2)=F(1)+F(30)+F(31)+F(32)
      MF(1,2)=(F(1)*MF(1,1)+F(30)*MF(1,30)+MF(1,32)*F(32)+F(31)*MF(1,31)
     C)/F(2)
      MF(2,2)=(F(30)*MF(2,30)+F(31)*MF(2,31)+F(32)*MF(2,32))/F(2)
      MF(3,2)=(F(30)*MF(3,30)+F(31)*MF(3,31)+F(32)*MF(3,32))/F(2)
      F(3)=F(2)*ALPH3
      F(4)=F(3)
      F(5)=F(2)-F(3)
      F(7)=F(4)*ALPH7
      F(6)=F(4)-F(7)
      F(8)=F(6)+F(5)
      F(9)=F(8)
      CALL MFRAC(5,2)
      CALL MFRAC(3,2)
      K11=EXP(33.334-20.0/(R*(T(4)+273.)))
      K12=EXP(33.334-20.0/(R*(T(9)+273.)))
      K21=EXP(37.94 -25.0/(R*(T(4)+273.)))
      K22=EXP(37.94 -25.0/(R*(T(9)+273.)))
      XA1=1-(1/(1+K11*TAU1))
      XB1=1-(1/(1+K21*TAU1))
      XA2=1-(1/(1+K12*TAU2))
      XB2=1-(1/(1+K22*TAU2))
      MF(1,4)=MF(1,2)*(1-XA1)
      MF(2,4)=(MF(2,2)+MF(1,2)*XA1)*(1-XB1)
      MF(3,4)=(MF(2,2)+MF(1,2)*XA1)*(XB1)+MF(3,2)
      CALL MFRAC(6,4)
      CALL MFRAC(7,4)
```

```
      MF(1,8)=(MF(1,6)*F(6)+MF(1,5)*F(5))/F(8)
      MF(2,8)=(MF(2,6)*F(6)+MF(2,5)*F(5))/F(8)
      MF(3,8)=(MF(3,6)*F(6)+MF(3,5)*F(5))/F(8)
      MF(1,9)=MF(1,8)*(1-XA2)
      MF(2,9)=(MF(2,8)+MF(1,8)*XA2)*(1-XB2)
      MF(3,9)=(MF(2,8)+MF(1,8)*XA2)*XB2+MF(3,8)
      F(10)=F(7)+F(9)
      MF(1,10)=(F(9)*MF(1,9)+F(7)*MF(1,7))/F(10)
      MF(2,10)=(F(9)*MF(2,9)+F(7)*MF(2,7))/F(10)
      MF(3,10)=(F(9)*MF(3,9)+F(7)*MF(3,7))/F(10)
      F(11)=F(10)
      CALL MFRAC(11,10)
      CALL MFRAC(34,38)
      CALL MFRAC(14,34)
      NMFA12=MF(1,10)
      NMFB12=MF(2,10)
      NF12=F(11)
      FOUND(1)=NF12
      FOUND(2)=NMFA12
      FOUND(3)=NMFB12
      GO TO 11
11    RETURN
      END
C     ******************************************************************
         SUBROUTINE DISTIL(SPLIT,F1,MFA1,MFB1,MFC1,SH,SL, EVOL1, EVOL2,
     CEVOL3,RRM, F2,F3,L,V,LB,VB,MFA2,MFB2,MFC2,MFA3,MFB3,MFC3,JA,COLUMN
     C)
      COMMON/RS/R1,R2,RM1,RM2
      COMMON/FUNDIS/ REVOL1,REVOL2,REVOL3
      INTEGER SPLIT
      REAL F1,MFA1, MFB1,MFC1,SH,SL,REVOL1,REVOL2,REVOL3,RRM,F2,F3,L,V,L
     CB,VB,MFA2,MFB2,MFC2,MFA3,MFB3,MFC3,JA
         IF(SPLIT.EQ.1) GO TO 100
         MFA3=0
         F3=SL*F1*MFB1+SH*F1*MFC1
         F2=MFA1*F1+(1-SL)*F1*MFB1+(1-SH)*F1*MFC1
         MFB3=SL*F1*MFB1/F3
         MFC3=SH*F1*MFC1/F3
         MFA2=MFA1*F1/F2
         MFB2=(1-SL)*F1*MFB1/F2
         MFC2=(1-SH)*F1*MFC1/F2
100      IF(SPLIT.EQ.2) GO TO 200
      MFC2=0
      F3=SL*F1*MFA1+F1*MFB1*SH+F1*MFC1
      F2=(1-SL)*F1*MFA1+(1-SH)*F1*MFB1
      MFA3=(SL*F1*MFA1)/F3
      MFA2=(1-SL)*F1*MFA1/F2
      MFB3=SH*F1*MFB1/F3
      MFB2=(1-SH)*F1*MFB1/F2
      MFC3=F1*MFC1/F3
200   CONTINUE
      RM=(MFA2*REVOL1/(REVOL1-JA)+MFB2*REVOL2/(REVOL2-JA)+MFC2*REVOL3/(
     CREVOL3-JA))-1.0
         R=RRM*RM
      IF(COLUMN.EQ.1) GO TO 16
      R2=R
      RM2=RM
      GO TO 17
16    CONTINUE
      RM1=RM
```

```
      R1=R
17       L=R*F2
         V=F2+L
         VB=V
         LB=F1+L
      RETURN
      END
C*********************************************************************
      FUNCTICN FUNCJ(I,ISTR)
      COMMON/CCMON/F,MF,T
      CCMMON/FUNDIS/ REVOL1,REVOL2,REVOL3
      REAL  CP,F(41),MF(3,41),T(41),CPA,CPB,CPC
      THA1=1.001
      IF(I.EQ.2) GO TO 40
      REVOL1=5.0
      REVOL2=1.0
      REVOL3=0.238
      THA2=4.999
      GO TO 50
40    REVOL1=21.0
      REVOL2=4.2
      REVOL3=1.0
      THA2=4.199
50     ZERO1=(((REVOL1*MF(1,ISTR))/(REVOL1-THA1)+
     C(REVOL2*MF(2,ISTR))/(REVOL2-THA1)+
     C(REVOL3*MF(3,ISTR))/(REVOL3-THA1)))
       ZERO2=(((REVOL1*MF(1,ISTR))/(REVOL1-THA2)+
     C(REVOL2*MF(2,ISTR))/(REVOL2-THA2)+
     C(REVOL3*MF(3,ISTR))/(REVOL3-THA2)))
20     THA3=(THA1+THA2)/2.
       ZERO3=(((REVOL1*MF(1,ISTR))/(REVOL1-THA3)+
     C(REVOL2*MF(2,ISTR))/(REVOL2-THA3)+
     C(REVOL3*MF(3,ISTR))/(REVOL3-THA3)))
      IF(ABS(THA1-THA2).LT.0.100) GO TO 30
      IF(ZERC1*ZERO3.LT.0.0) GO TO 10
      THA1=THA3
      ZERO1=ZERO3
      GO TO 20
10    THA2=THA3
      ZERO2=ZERC3
      GO TO 20
30    FUNCJ=THA3
      RETURN
      END
C      ***************************************************************
      SUBROUTINE COSCAL(PFUNC,JOB)
      INTEGER DEPRCI,PROFUN
      REAL F(41),MF(3,41),T(41),JA1,JA2,MWA,MWB,MWC,IT,K11,K12,K21,K22,
     CN1,N2,NM1,NM2,LDELT1,LDELT2,LDELT3,LDELT4,LDELT5,LDELT6,LDELT7,
     CLDELT8,LDELT9,MSX
      COMMON/COMON/F,MF,T
      CCMMON/STRPRM/ALPH3,ALPH7,ALPH36,ALPH14,ALPH23,ALPH25,ALPH26,T2,T4
     C,T9,T11,TAU1,TAU2,S1L,S1H,S2L,S2H,RRM1,RRM2,PICK,CT11
      CCMMON/CAT/ MSX,ENRX,DEPRCI,PROFUN,CONI,TAXRAT
      CCMMON/XXX/K11,K12,K21,K22,XA1,XA2,XB1,XB2
      COMMON/RS/R1,R2,RM1,RM2
      CCMMCN/COM/B,A,NN
      INTEGER A,B
      IF(JOB.NE.1) GO TO 20
      UFLWE3=0.
```

```
      UCOSE3=0.C
      REVOLA=21.0
      REVOLB=4.2
      REVOLC=1.0
      HA=7.36
      HB=8.73
      HC=9.4
      MWA=78.11
      MWB=112.51
      MWC=147.01
      CPW=0.018
      HS=11.73
      CPA=0.0325
      CPB=0.03585
      CPC=0.0342
      TI=20.0
      TO=30.
      DH1=-60.
      DH2=-30.0
      TS=174.0
      TA=80.1
      TB=132
      TC=174
      WCOST=0.0000003366
      SCOST=0.0000436
      LAMDA=0.10
      MU=0.25
      BETA=0.5
      UCOOL=200
      UCOND=300
      RHOA=879000
      RHOB=1110000
      RHOC=1530000
      TRAYSP=0.5
      RMCOST=4031520
      R=0.000082
      T(1)=20.0
      F(1)=55233
      IF(JOB.EQ.1) RETURN
20    T(12)=TA*MF(1,12)+TB*MF(2,12)+TC*MF(3,12)
      T(16)=TA*MF(1,16)+TB*MF(2,16)+TC*MF(3,16)
      T(38)=TA*MF(1,38)+TB*MF(2,38)+TC*MF(3,38)
      T(19)=TA*MF(1,19)+TB*MF(2,19)+TC*MF(3,19)
      T(41)=TA*MF(1,41)+TB*MF(2,41)+TC*MF(3,41)
      T(39)=TA*MF(1,39)+TB*MF(2,39)+TC*MF(3,39)
      T(36)=T(16)
      T(35)=T(38)
      T(22)=T(41)
      T(33)=T(39)
      T(20)=T(39)
        T(17)=T(16)
        T(34)=T(38)
        T(15)=T(38)
        T(14)=T(38)
      T(5)=T(2)
      T(3)=T(2)
      T(13)=T(16)
      T(18)=T(16)
      T(37)=T(16)
      T(40)=T(41)
```

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      T(21)=T(41)
        T(6)=T(4)
        T(7)=T(4)
        T(23)=T(41)
        T(22)=T(41)
        T(26)=T(23)
        T(24)=T(18)
        T(28)=(T(24)*CP(24)*F(24)+T(26)*CP(26)* F(26))/(F(28)*CP(28))
      T(10)=(F(7)*T(7)*CP(7)+F(9)*CP(9)*T(9))/(CP(10)*F(10))
      T(11)=T(10)+CT11*(T(28)-T(10))
      T(29)=(T(28)*CP(28)*F(28)-CP(10)*F(10)*(T(11)-T(10)))/(CP(28)*F(28
     C))
      T(8)=(F(5)*T(5)*CP(5)+F(6)*CP(6)*T(6))/(F(8)*CP(8))
      T(31)=(T(2)*CP(2)*F(2)-T(1)*F(1)*CP(1))/(F(31)*CP(31)+CP(30)*F(30)
     C+CP(32)*F(32))
      T(30)=T(31)
      IF(T(29).LT.T(30)) GO TO 30
      GO TO 29
30    T(29)=T(30)
      T(11)=(T(10)*F(10)*CP(10)+T(28)*F(28)*CP(28)-T(29)*F(29)*CP(29))
     C/(F(11)*CP(11))
29    CONTINUE
      T(32)=T(30)
        T(24)=T(18)
        T(27)=T(23)
        T(25)=T(18)
      Q1=CP(27)*F(27)*ABS(T(27)-T(31))
      Q2=CP(25)*F(25)*ABS(T(25)-T(32))
      Q3=CP(28)*F(28)*ABS(T(28)-T(29))
      Q4=CP(29)*F(29)*(T(29)-T(30))
      IF(T(29) .LT.T(30)) Q4=0.0
C       ***********  CHECK T(11)=T(29)
      Q5=CP(10)*F(10)*(T(12)-T(11))
      Q6=(HA*MF(1,16)+HB*MF(2,16)+HC*MF(3,16))*F(16)
      Q7= (HA*MF(1,35)+HB*MF(2,35)+HC*MF(3,35))*F(35)
      Q8= (HA*MF(1,41)+HB*MF(2,41)+HC*MF(3,41))*F(41)
      Q9= (HA*MF(1,33)+HB*MF(2,33)+HC*MF(3,33))*F(33)
      LDELT1=((T(27)-TO)-(T(31)-TI))/ALOG(ABS((T(27)-TO)/(T(31)-TI)) )
      AREAE1=Q1/(UCOOL*LDELT1)
      LDELT2=((T(25)-TO)-(T(32)-TI))/ALOG(ABS((T(25)-TO)/(T(32)-TI)) )
      AREAE2=Q2/(UCOOL*LDELT2)
       IF(T(28)-T(11).GT.0.AND.T(29)-T(10).GT.0) GO TO 52
      AREAE3=0
       GO TO 53
52    CONTINUE
      LDELT3=((T(28)-T(11))-(T(29)-T(10)))/ALOG((T(28)-T(11))/(T(29)-T(1
     C0)))
      AREAE3=Q3/(UCOOL*LDELT3)
53     CONTINUE
      IF(T(29).LT.TO)AREAE4=0.000000001
      IF(T(29).LT.TO)  GO TO 231
      LDELT4=((T(29)-TO)-(T(30)-TI))/ALOG((T(29)-TO)/(T(30)-TI))
      AREAE4=Q4/(UCOOL*LDELT4)
231   CONTINUE
      LDELT5=((TS-T(11))+(TS-T(12)))/2
      AREAE5=Q5/(UCOND*LDELT5)
      LDELT6=((T(16)-TI)+(T(16)-TO))/2
      AREAE6=Q6/(UCOND*LDELT6)
      LDELT7=(TS-T(35))
      AREAE7=Q7/(UCOND*LDELT7)
```

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      LDELT8=((T(41)-TI)+(T(41)-TO))/2
      AREAE8=Q8/(UCOND*LDELT8)
      LDELT9=TS-T(33)
      AREAE9=Q9/(UCOND*LDELT9)
      UFLWR1=(CP(3)*F(3)*T(3)-CP(4)*F(4)*T(4)-(XA1*F(3)*MF(1,3)*DH1+XA1
     C*XB1*F(3)*MF(1,3)*DH2+XB1*F(3)*MF(2,3)*DH2))/(CPW*(TO-TI))
      UFLWR2=(CP(8)*F(8)*T(8)-CP(9)*F(9)*T(9)-( XA2*F(8)*MF(1,8)*DH1+
     CXA2*XB2*F(8)*MF(1,8)*DH2+XB2*F(8)*MF(2,8)*DH2))/(CPW*(TO-TI))
      UFLWE1=Q1/((TO-TI)*CPW)
      UFLWE2=Q2/((TO-TI)*CPW)
      UFLWE4=Q4/((TO-TI)*CPW)
      UFLWE5=Q5/HS
      UFLWE6=Q6/((TO-TI)*CPW)
      UFLWE8=Q8/((TO-TI)*CPW)
      UFLWE7=Q7/HS
      UFLWE9=Q9/HS
      D=F(16)-F(36)
      TC1=(T(16)+T(38))/2+273
      IF(PICK.LT.0.5          ) GO TO 500
      RELVA=(REVOLC*REVOLB)**0.5
      SL=1- (D*MF(2 ,16)/(F(12)*MF(2 ,12)))
      SH=1- (D*MF(3 ,16)/(F(12)*MF(3 ,12)))
500   IF(PICK.GE.0.5          ) GO TO 600
      RELVA=((REVOLB/REVOLB)*(REVOLA/REVOLB))**0.5
      SL=1- (D*MF(1 ,16)/(F(12)*MF(1 ,12)))
      SH=1- (D*MF(2 ,16)/(F(12)*MF(2 ,12)))
600   NM1=ALOG(((1-SL)/SL)*(SH)/(1-SH))/ALOG(RELVA)
      JA1=2.3*(-0.9*((R1-RM1)/(R1+1)) -0.17)
      N1=(NM1+EXP(JA1))/(1-EXP(JA1))
      IF(N1.LT.1.0)  N1=1
       DIAM1=SQRT((4*F(35)*TC1*R)/(3600*3.14159))
      CTRAY1=70*(N1/0.5)*(DIAM1*10.764/4.0)**1.9
      CTOW1=4.34*2500*DIAM1*10.764*((N1+1.)*3.28*TRAYSP/40.)**0.68
      COSTD1= CTOW1+CTRAY1
      D=F(41)-F(22)
      TC2=(T(41)+T(39))/2+273
      IF(PICK.GE.0.5          ) GO TO 700
      RELVA=(REVOLC*REVOLB)**0.5
      SL=1- (D*MF(2 ,41)/(F(19)*MF(2 ,19)))
      SH=1- (D*MF(3 ,41)/(F(19)*MF(3 ,19)))
700   IF(PICK.LT.0.5          ) GO TO 800
      RELVA=((REVOLB/REVOLB)*(REVOLA/REVOLB))**0.5
      SL=1- (D*MF(1 ,41)/(F(19)*MF(1 ,19)))
      SH=1- (D*MF(2 ,41)/(F(19)*MF(2 ,19)))
800   JA2=2.3*(-0.9*((R2-RM2)/(R2+1))-0.17 )
      NM2=ALOG(((1-SL)/SL)*(SH)/(1-SH))/ALOG(RELVA)
      N2=(NM2+EXP(JA2))/(1-EXP(JA2))
      IF(N2.LT.1.0) N2=1
       DIAM2=SQRT((4*F(33)*TC2*R)/(3600*3.14159))
      CTRAY2=70*(N2/0.5)*(DIAM2*10.764/4.0)**1.9
      CTOW2=4.34*2500*DIAM2*10.764*((N2+1.)*3.28*TRAYSP/40.)**0.68
      COSTD2= CTOW2+ CTRAY2
      VLOWP1=F(2 )*(MF(1,2 )*MWA*(1/RHOA)+MF(2,2 )*MWB*(1/RHOB)+MF(3, 2)
     C*MWC*(1/RHOC))
      VLOWP2=F(4 )*(MF(1,4 )*MWA*(1/RHOA)+MF(2,4 )*MWB*(1/RHOB)+MF(3,4 )
     C*MWC*(1/RHOC))
      VLOWP3=F(9 )*(MF(1,9 )*MWA*(1/RHOA)+MF(2, 9)*MWB*(1/RHOB)+MF(3,9 )
     C*MWC*(1/RHOC))
      VLOWP4=F(38)*(MF(1,38)*MWA*(1/RHOA)+MF(2,38)*MWB*(1/RHOB)+MF(3,38)
     C*MWC*(1/RHOC))
```

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      VLOWP5=F(16)*(MF(1,16)*MWA*(1/RHOA)+MF(2,16)*MWB*(1/RHOB)+MF(3,16)
     C*MWC*(1/RHOC))
      VLOWP6=F(39)*(MF(1,39)*MWA*(1/RHOA)+MF(2,39)*MWB*(1/RHOB)+MF(3,39)
     C*MWC*(1/RHOC))
      VLOWP7=F(41)*(MF(1,41)*MWA*(1/RHOA)+MF(2,41)*MWB*(1/RHOB)+MF(3,41)
     C*MWC*(1/RHOC))
      RMCOST=4031520
      PRODM=AMAX1(                    MF(2,14),MF(2,13))
      IF(PRODM.EQ.MF(2,14)) PRODT=MF(2,14)*F(14)
      IF(PRODM.EQ.MF(2,13)) PRODT=MF(2,13)*F(13)
      SALES=8400.*(14.9/100000.)*MWA*PRODT
      IF(AMAX1(MF(2,13),MF(2,14),MF(2,20),MF(2,40)).LT.0.95) GO TO 776
      PROD=F(13)+F(14)+F(20)+F(40)
      IF(MF(2,13).LT.0.95) PROD=PROD-F(13)
      IF(MF(2,14).LT.0.95) PROD=PROD-F(14)
      IF(MF(2,20).LT.0.95) PROD=PROD-F(20)
      IF(MF(2,40).LT.0.95) PROD=PROD-F(40)
      SALES=8400.*(14.9/100000.)*PROD*MWA
776   CONTINUE
      COSTE1=726.+566.*(AREAE1/0.09)**0.61
      COSTE2=726.+566.*(AREAE2/0.09)**0.61
      COSTE3=726.+566.*(AREAE3/0.09)**0.61
      COSTE4=726.+566.*(AREAE4/0.09)**0.61
      COSTE5=726.+566.*(AREAE5/0.09)**0.61
      COSTE6=37290.*(AREAE6*0.01076)**0.65
      COSTE7=37290.*(AREAE7*0.01076)**0.65
      COSTE8=37290.*(AREAE8*0.01076)**0.65
      COSTE9=37290.*(AREAE9*0.01076)**0.65
      COSTR1=520.+436.*(TAU1*F(3)*(MF(1,3)*MWA*(1/RHOA)+MF(2,3)*MWB*(1./
     CRHOB)+MF(3,3)*MWC*(1./RHOC))*264   )**0.61+726.+700.*(UFLWR1*CPW*(T
     CO-TI)/((((T(3)-TO)+(T(4)-TI))/2)*UCOOL))**0.61
      COSTR2=520.+436.*(TAU2*F(8)*(MF(1,8)*MWA*(1/RHOA)+MF(2,8)*MWB*(1./
     CRHOB)+MF(3,8)*MWC*(1./RHOC))*264. )**0.61+726.+700.*(UFLWR2*CPW*(T
     CO-TI)/((((T(8)-TO)+(T(9)-TI))/2)*UCOOL))**0.61
      COSTP1=215.*(VLOWP1*4.4028)**0.6
      COSTP2=215.*(VLOWP2*4.4028)**0.6
      COSTP3=215.*(VLOWP3*4.4028)**0.6
      COSTP4=215.*(VLOWP4*4.4028)**0.6
      COSTP5=215.*(VLOWP5*4.4028)**0.6
      COSTP6=215.*(VLOWP6*4.4028)**0.6
      COSTP7=215.*(VLOWP7*4.4028)**0.6
      UCOSR1=UFLWR1*WCOST
      UCOSR2=UFLWR2*WCOST
      UCOSE1=UFLWE1*WCOST
      UCOSE2=UFLWE2*WCOST
      UCOSE4=UFLWE4*WCOST
      UCOSE5=UFLWE5*SCOST
      UCOSE6=UFLWE6*WCOST
      UCOSE7=UFLWE7*SCOST
      UCOSE8=UFLWE8*WCOST
      UCOSE9=UFLWE9*SCOST
      UCOSUT=UCOSR1+UCOSR2+UCOSE1+UCOSE2        +UCOSE4+UCOSE5+UCOSE6+UCO
     CSE7+UCOSE8+UCOSE9
      COSTRT=COSTR1+COSTR2
      COSTET=COSTE1+COSTE2+COSTE3+COSTE4+COSTE5+COSTE6+COSTE7+COSTE8+COS
     CTE9
      COSTPT=COSTP1+COSTP2+COSTP3+COSTP4+COSTP5+COSTP6+COSTP7
      COSTDT=COSTD1+COSTD2
      IT=COSTRT+COSTET+COSTPT+COSTDT
      CIX=IT*((MSX/330.0)*(1.-.3)+.3*(ENRX/1774.))
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      ZIN=CONI*11.0
      EXPMIN=1.-EXP(-ZIN)
      IF(DEPRCI.EQ.1) RTAX=(CIX/11.)*((ZIN/EXPMIN)-TAXRAT)
      IF(DEPRCI.EQ.2) RTAX=(CIX/11.)*((ZIN/EXPMIN)-(2.*TAXRAT/EXPMIN)
     C+(2.*TAXRAT/ZIN))
      P=(SALES-RMCOST-UCOSUT*8400.)*(1.-TAXRAT)-RTAX
      IF(PROFUN.EQ.1) PFUNC=P
      IF(PROFUN.EQ.2) PFUNC=P/CIX*100.
      IF(PROFUN.EQ.3) PFUNC=CIX/SALES
      IF(PROFUN.EQ.4) PFUNC=(SALES-RMCOST-UCOSUT*8400.)*(1.-TAXRAT)-
     CC.25*CIX
      UNIFLW=P
      RATER=P/CIX*100.
      PAYOUT=CIX/P
      VENPRF=(SALES-RMCOST-UCOSUT*8400.)*(1.-TAXRAT)-0.25*CIX
      IF(JOB.EQ.2) RETURN
      WRITE(6,320)
320   FORMAT('1' ,T60,'** FLOW MATRIX **')
      WRITE(6,110)
110   FORMAT('0', 22X,'STREAM  FLOW RATE(GMOLES/HR)',5X,'%A',14X,'%B',13
     CX,'%C',8X,'TEMP (DEGREE C)')
      DO 32 I123=1,41,1
      WRITE(6,120)I123,F(I123),MF(1,I123),MF(2,I123),MF(3,I123),T(I123)
120   FORMAT(' ',T25,I2,T35,F8.1,T53,E13.7,T68,E13.7,T83,E13.7,T102,F6.2
     C)
32    CONTINUE
       WRITE(6,400)
400    FORMAT('1', T60,'** DATA MATRIX **')
       WRITE(6,857)
       WRITE(6,410)  K11,K12
410    FORMAT(' ','K1',T13,2(E11.4,1X))
       WRITE(6,420)  K21,K22
420    FORMAT(' ','K2',T13,2(E11.4,1X))
       WRITE(6,430)  XA1,XA2
430    FORMAT(' ','XA',T13,2(F11.9,1X))
       WRITE(6,440)  XB1,XB2
440    FORMAT(' ','XB',T13,2(F11.8,1X))
       WRITE(6,450) UFLWR1,UFLWR2
450    FORMAT(' ','U R FLW'        ,T13,2(F11.0,1X))
       WRITE(6,460) RM1,RM2
460    FORMAT(' ','MIN REFLUX',T13,2(F11.2,1X))
       WRITE(6,470) R1,R2
470    FORMAT(' ','REFLUX RATIO',T13,2(F11.2,1X))
       WRITE(6,480) NM1,NM2
480    FORMAT(' ','MIN TRAYS',T13,2(F11.2,1X))
       WRITE(6,490) N1,N2
490    FORMAT(' ','NUMBER TRAYS',T13,2(F11.2,1X))
      WRITE(6,411) DIAM1,DIAM2
411   FORMAT(' ','DIAMETERS ',T13,2(F11.2,1X))
       WRITE(6,501)Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9
501    FORMAT(' ','HEAT EXCH LD'  ,T13,9(F11.2,1X))
       WRITE(6,510) LDELT1,LDELT2,LDELT3,LDELT4,LDELT5,LDELT6,LDELT7,
     CLDELT8,LDELT9
510    FORMAT(' ','EXCH DEL TEMP',T13,9(F11.2,1X))
       WRITE(6,520) AREAE1,AREAE2,AREAE3,AREAE4,AREAE5,AREAE6,AREAE7,
     CAREAE8,AREAE9
520    FORMAT(' ','EXCH AREA',T13,9(F11.2,1X))
       WRITE(6,530) UFLWE1,UFLWE2,UFLWE3,UFLWE4,UFLWE5,UFLWE6,UFLWE7,
     CUFLWE8,UFLWE9
530    FORMAT(' ','EXCH UTIL FLW' ,T13,9(F11.0,1X))
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      WRITE(6,540) VLCWP1,VLOWP2,VLOWP3,VLOWP4,VLOWP5,VLOWP6,VLOWP7
540   FORMAT(' ','PUMP FLOW RATE',T13,7(F11.2,1X))
      WRITE(6,330)
330   FORMAT('0',T63,'** COST MATRIX **')
      WRITE (6,857)
857   FORMAT ('0','UNIT NO.',T19,'1',T33,'2',T45,'3',T57,'4',T69,'5',T81
     C,'6',T93,'7',T105,'8',T117,'9')
      WRITE(6,121) COSTE1,COSTE2,COSTE3,COSTE4,COSTE5,COSTE6,COSTE7,
     CCOSTE8,COSTE9
121   FORMAT(' ','H EXCH',T13,9(F11.2,1X))
      WRITE(6,130)COSTP1,COSTP2,COSTP3,COSTP4,COSTP5,COSTP6,COSTP7
130   FORMAT(' ','PUMP',T13,7(F11.2,1X))
      WRITE(6,140)COSTR1,COSTR2
140   FORMAT(' ','REACTOR',T13,2(F11.2,1X))
      WRITE(6,150)CTRAY1,CTRAY2
150   FORMAT(' ','TRAY',T13,2(F11.2,1X))
      WRITE(6,160)CTCW1,CTCW2
160   FORMAT(' ','TOWER',T13,2(F11.2,1X))
      WRITE(6,170)COSTD1,COSTD2
170   FORMAT(' ','COLUMN',T13,2(F11.2,1X))
      WRITE(6,180)UCOSE1,UCOSE2,UCOSE3,UCOSE4,UCOSE5,UCOSE6,UCOSE7,UCOSE
     C8,UCOSE9
180   FORMAT(' ','UTIL H EXCH',T13,9(F11.2,1X))
      WRITE(6,190)UCOSR1,UCOSR2
190   FORMAT(' ','UTIL REACTOR',T13,2(F11.2,1X))
      WRITE(6,310)
310   FORMAT(' ',T64,'TOTAL COSTS')
      WRITE(6,210)UCOSUT
210   FORMAT(' ','UTIL TOTAL ($/HR)',T64,F11.2)
      WRITE(6,220)SALES
220   FORMAT(' ' ,'SALES ($/YEAR)',T64,F11.2)
      WRITE(6,230)RMCOST
230   FORMAT(' ','RM COST ($/YEAR)',T64,F11.2)
      WRITE(6,240)IT
240   FORMAT(' ' ,'INVESTMENT ($)',T64,F11.2)
      WRITE(6,99) PFUNC
99    FORMAT(' ','PROFIT FUNC ($) = ',T64,F11.2)
      WRITE(6,991) UNIFLW
991   FORMAT(' ','UNIFLOW ($) = ',T64,F11.2)
      WRITE(6,992) RATER
992   FORMAT(' ','RATE OF RETURN (%) = ',T64,F11.2)
      WRITE(6,993) PAYOUT
993   FORMAT(' ','PAY OUT TIME (YEARS) = ',T64,F11.2)
      WRITE(6,994) VENPRF
994   FORMAT(' ','VENTURE PROFIT ($) = ',T64 ,F11.2)
      GO TO 11
11    RETURN
      END
$ENTRY
$STOP
```

APPLICATIONS OF SYSTEMS SYNTHESIS

TECHNIQUES TO INDUSTRIAL SYSTEMS

by

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B. S., Kansas State University, 1973

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY

Manhattan, Kansas

1975

ABSTRACT

The methods of systems synthesis have been applied to the design of nonlinear, nonserial, heterogeneous systems in order to judge the ease of application, efficiency, and accuracy of each technique.

An extensive review of the most recent methods and applications of systems synthesis was conducted to isolate those synthesis methods which could be considered applicable to the design of nonlinear, nonserial, heterogeneous systems.

A cooling system used in the power generation industry and a complex chemical plant were designed with several of the most promising synthesis techniques. The results of this study indicate that the "Heuristic Technique" and direct search with a structural parameter solution formulation may be the only methods applicable to nonlinear, nonserial, heterogeneous systems synthesis. An evolutionary approach should be considered along with the direct search of the structural parameter method of preliminary engineering judgement needed for the structural parameter solution formulation.