MIXED-INTEGER PROGRAMMING: IS IT A USEFUL TOOL IN PROCESS SYNTHESIS?

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Abstract

This paper deals with the problem of developing algorithmic methods for synthesizing chemical processes. It is shown that mixed-integer programming is the natural underlying tool for these type of methods. Mixed- integer linear programming models are reviewed for utility systems, heat recovery networks, integrated refrigeration systems and total processing systems. Specific examples are presented to show the versatility and scope of these type of techniques, as well as the shortcomings when other approaches are used. A brief outline for handling explicitly nonlinearities is also presented.

Scope

Process synthesis is one of the most important areas within Chemical Process Design since it deals with the problem on how to integrate process flowsheets for manufacturing chemical products. Ideally the objective is to derive flowsheet structures that are economically attractive, energy efficient, and which at the same time exhibit good operability characteristics such as flexibility, resiliency, reliability and safety. Although some progress has been made recently in incorporating the latter objectives (see Grossmann and Morari, 1983), most of the previous work has concentrated on the economic objective since this is one of the primary goals at the initial stages of design.

Over the last fifteen years a major research effort has been undertaken to study and understand the activity of process synthesis. Extensive reviews on the subject can be found in Hendry et al (1973), Hlavacek (1977), Westerberg (1980), Stephanopoulos (1981) and Nishida et al (1981). Due to the fact that synthesis problems are combinatorial and open-ended in nature a number of different approaches have been proposed for synthesis problems. These approaches can be classified in heuristics, thermodynamic targets and algorithmic methods that are based mainly on optimization techniques. In the recent past it is the first two approaches that have received most of the attention due to apparent limitations and failures with optimization techniques.

It is the purpose of this paper to show that algorithmic methods can indeed play a very useful role in process synthesis. In particular, it will be shown that mixed-integer programming is the natural tool for algorithmic methods. A number of applications developed by our research group at Carnegie-Mellon University will be discussed. Rather than emphasizing the mathematical formulations which can be found in previous publications, examples will be presented to show the versatility of mixed-integer programming and its great potential for synthesizing integrated total processing systems in which interactions are explicitly taken into account. These examples will also show the shortcomings of heuristics and simple minded decomposition schemes. Furthermore, the proper combination or blend of the three basic approaches for process synthesis will be discussed.

Conclusions and Significance

This paper has attempted to show how algorithmic methods can play a useful role in process synthesis together with the heuristic and thermodynamic approaches. Furthermore, it has been shown that mixed-integer programming is the underlying tool for algorithmic methods. Apart from providing a common mathematical framework for solving a variety of synthesis problems, the advantage with mixed-integer programming is that it provides a natural way of accounting explicitly for the interactions in integrated flowsheets that are composed of several major components. These points have been illustrated in the following synthesis problems: utlility systems, heat recovery networks, integrated refrigeration systems and total processing systems. Results of the example problems have shown not only that the solutions can be obtained with reasonable computational expense, but that very often these solutions are much more economical than when problems are decomposed in an ad hoc fashion. Finally, an outline of a promising algorithm that can account for nonlinearties has been discussed.

Introduction

The three major approaches that have been proposed in process synthesis in order to integrate process flowsheets can be summarized as follows:

1. Heuristics. Here the main idea is to apply rules of thumb that are based on engineering judgement or experience (see Masso and Rudd, 1969; Douglas, 1982). The advantage with heuristics is that they allow to find very quickly flowsheet structures that often are "near" optimal solutions. However, the drawback is that usually there is no reasonable way to establish the quality of such solutions which sometimes can in fact be rather poor. Furthermore, heuristic rules for a given problem may often contradict each other which then requires the assignment of rather arbitrary rankings or weighting schemes to resolve these conflicts.

2. Thermodynamic targets. The main conjecture in this approach is that designs featuring high energy efficiency are very often "near" optimal solutions from an economic viewpoint. By performing a thermodynamic analysis one can often derive lower bounds on energy consumption which then provide targets for the design engineers (e.g. see Linnhoff et al. 1982). Clearly, this approach can be very powerful in reducing the combinatiorial problem if the quality of the bounds is very good (e.g. minimum utility consumption in heat recovery networks; Hohmann, 1971, Linnhoff and Flower, 1978), and if energy is in fact a dominant cost item in the process. The main drawback in this approach is that capital cost considerations cannot be properly accounted for since this can only be done by artifically restricting the energy efficiency (e.g. through min temperature approaches). Also, since targets provide only guidelines, considerable insight and trial and error may be required from the design engineer to find solutions that are close to the predicted targets.

3. Algorithmic. The main idea in this approach is to.formulate the synthesis of a flowsheet as an optimization problem (e.g. see Umeda et al. 1972; Papoulias and Grossmann, 1983 a,b,c). This requires an explicit or implicit representation of a specified set of flowsheets among which the optimal solution will be selected. The advantage in this approach is that it provides a more systematic framework for handling a variety of process synthesis problems, and for accounting more rigorously for features such as interactions and capital costs. Also, this approach has the important property of being able to generate automatically flowsheet structures. The disadvantage however, is that the computational expense can be rather large when problems are not properly formulated, and furthermore, optimality of the solutions can only be guaranteed with respect to the alternatives that have been considered in the problem representation.

It should be pointed out that the distinction between the three approaches is obviously not always clear cut. For* instance, both thermodynamic and algorithmic methods make use of heuristics in one way or another, whereas some of the heuristic methods are to some extent algorithmic in the sense that they can be systematyzed (e.g. through expert systems, see Hart, 1983).

Recently, there has been considerable skepticism on the usefulness of algorithmic methods that are based on optimization. The main arguments against the use of these methods for process synthesis can be summarized as follows:

1. They remove design engineers from the decision making process
2. They provide little insights as to why decisions are made
3. They tend to be computationally expensive
4. They cannot guarantee "true" optimality because of the many intangibles in design, or because alternatives that are potentially better may not have been included in the problem representation.

While there is no denial that these objections have some validity, it is also true that they tend to arise because of misconceptions and lack of appreciation of the capabilities and limitations that optimization techniques have. In particular, the main problem would seem to be on how algorithmic methods should fit in relation to the two other approaches in process synthesis.

Although there is no question that considerable progress has been made in process synthesis with heuristics and thermodynamic targets (see Stephanopoulos, 1981), particularly with heat recovery networks, it is also true that these methods have a number of important limitations. For instance, these methods do not provide a common framework for synthesizing a variety of systems or total processing systems that are composed of different types of major components (e.g. chemical plant, heat integration network, utility systems). Also, heuristics and thermodynamic targets tend to leave all the synthesis decisions to the engineer which can make them rather cumbersome and tedious when applied to large systems. Finally, these methods can also fail to guarantee "true" optimality, either because they tend to make rather restrictive assumptions (e.g. neglect of capital cost considerations, dominance of energy considerations), or because they are subject to the particular interpretation and skill of the design engineer in their application.

Since neither heuristics, thermodynamic targets or algorithmic methods would appear to offer by themselves the single "right" way to tackle process synthesis problems, a more sensible strategy would seem to be to combine the three approaches so as to exploit their respective strengths. For instance, heuristics could be used in preliminary screening to eliminate alternatives that are likely not to be promising, or else they could be used to generate "good" initial estimates. Thermodynamic targets could be used to develop bounds or representations that will eliminate from consideration alternatives that are not energy efficient. Algorithmic methods could be used to automatically generate integrated flowsheets in which the interactions and finer modelling points are taken fully into account.

In this way, by properly blending the three approaches within an interactive computing environment the design engineer could still be in full command of the decision process. By developing insights through heuristics and thermodynamic targets he could incorporate them into the algorithmic procedures, vyhile these in turn will aid the engineer in the search of minimum cost solutions. When these solutions do not prove to be satisfactory from a practical viewpoint, he could have the capability of either imposing additional constraints in the algorithmic methods, or else to make modifications to the flowsheet structure at his will. In summary, the motivation behind this scheme would be to expand the capabilities available to the engineer for synthesis rather than restricting him to either analysis programs in which he has to make all the synthesis decisions, or to automatic synthesis programs where he cannot effectively participate in the decision making process.

It is the purpose of this paper to demonstrate that algorithmic methods can indeed play a useful role in process synthesis provided that they are used within a framework as described above. In particular, this paper will show that mixed-integer programming is the natural underlying tool for algorithmic methods because it provides a general mathematical framework for process synthesis problems. These ideas will be illustrated through several example problems in the areas of utility systems, heat recovery networks, integrated refrigeration systems and total processing systems. These examples will also show that computational efficiency is possible witt* mixed-integer programming, and that it can avoid shortcomings associated with the use of heuristics and with simple minded decomposition schemes which may often overlook more economical solutions.

Mixed-integer programming

Mixed-integer programming deals with optimization techniques in which an objective function is optimized subject to both equality and inequality constraints, and where two types of variables can be specified: continuous variables which can take any real value within given bounds, and binary variables which can take only 0-1 values. The unique feature is precisely the capability of handling the latter type of variables which in application problems can be associated to discrete decisions.

In the context of process synthesis, the application of mixed- integer programming requires that a superstructure be postulated which has embedded many flowsheet alternatives that are to be analyzed. This superstructure, which must be specified by the design engineer, could in general be developed with the use of heuristics and thermodynamic targets. Continuous variables x can then be associated to flowrates, equipment sizes, pressures and temperatures, while 0-1 binary variables y can be associated to the existence of units that are postulated for the flowsheets in the superstructure. This then yields a problem of the form

$$\begin{aligned} &\min\ C=f(x,y) \\ &\text{s.t.}\ \ h(x,y) = 0 \\ &\qquad g(x,y) \le 0 \\ &xGR^{n}\ ,\ y€\{0,1\}^{m} \end{aligned} \tag{I}$$

where the objective function C=f(x,y) will in general represent a desired economic measure, while the equality and inequality constraints h(x,y), g(x,y), can be derived from the superstructure to represent heat and material balances, design equations.

physical constraints, design specifications or logical conditions that should be satisfied in the flowsheets.

The three major features of the mixed-integer programming problem in (I) for process synthesis are the following:

1. Structural and parameter optimization can be performed simultaneously. This is clearly a very important point since in process synthesis discrete decisions that are involved in the selection of a flowsheet also implies making continuous decisions such as in the selection of flowrates, equipment sizes, or levels of pressure and temperature which in some cases can have a very important effect on the structure.

2. Discrete and logical constraints can be handled explicitly with the binary variables. This feature, which overcomes a major limitation that continuous optimization procedures have (e.g. see Umeda et al,1972), is very powerful because it allows the designer to specify constraints or conditions that will yield realistic flowsheet structures.

3. The mathematical representation provides a general systematic framework since one can formulate a variety of different synthesis problems with the same mathematical tool. The importance of this feature lies on the fact that total processing systems (e.g. see Fig.l) can be synthesized by simply interconnecting the models for the different components. In this way interactions of the different subsystems can be be taken explicitly into account for the overall optimization.

Although from a conceptual viewpoint mixed-integer programming is the natural tool for algorithmic methods in process synthesis, it is well known that the corresponding techniques can be somewhat inefficient when the size of the problem is very large, particularly in regard to the number of binary variables. Therefore, to make this approach useful it is essential to overcome the two following problems:

1. Find an efficient representation for the superstructure which leads to problems of reasonable size.

2. Use or develop efficient optimization techniques that exploit the structure of the problems.

The first aspect is clearly problem dependent, and it is the one where heuristics and thermodynamic targets can play a very useful role. As for the second aspect,one has to realize that efficient algorithms for solving the problem in the general form of (I) are only available for two important cases. The first one is where problem (I) is reformulated to the form of a mixed-integer linear programming (MILP) problem, and the second case is when problem (I) is formulated as a mixed-integer nonlinear program (MINLP) in which the binary variables are linear and separable from the continuous variables which appear in nonlinear form. This paper will deal mainly with the former case, and a brief outline of some promising ideas for the latter case will be given at the end of this paper.

Mixed-integer linear programming is a class of problems for which the functions involved in problem (I) are linear. Efficient computer codes are available for large-scale MILP problems (see Geoffrion and Martsen,1972; Tomlin, 1982), and they have the important property of being able to determine global optimum solutions.

In order to convert the functions f, h, and g in problem (I) in linear forms, this can be accomplished by discretizing operating conditions such as pressures, temperatures, split fractions, with which linear equations can be derived for the performance of each unit (see Grossmann and Santibanez,1980; Papoulias and Grossmann, 1983a). The effect of operating conditions can then be analyzed by considering them through a set of discrete values with which linearity in the performance equations and constraints is maintained. To denote the existence or non-existence of each discrete operating condition at each unit, 0-1 variables can be introduced with the constraint that each unit can operate at most in one condition. The following variables can then be associated with the general superstructure:

1. The n_y - vector y of binary variables which indicate the existence or non-existence of units, and which define the flowsheet configuration of the process.

2. The n_y^d - vector y^d of binary variables which indicate the existence or non-existence of the discrete fixed operating conditions x^d that are to be analyzed.

3. The n_x^c - vector x^c of continuous variables which correspond to stream flowrates and sizes of units.

Therefore, the constraint set describing the performance of the general processing scheme in the steady-state can be represented by the system of linear equality and inequality constraints:

$$E_1 \, y^d + E_2 \, x^c = e \qquad (2)$$

$$d^L \le D_1 \, y + D_2 \, y^d + D_3 \, x^c \le d^U$$

where the matrices E_1 and D_2 are functions of the selected fixed operating conditions x^d.

The nonlinear objective function C can be approximated using fixed- charge cost functions. The actual investment cost function for a plant unit is commonly a concave cost function as shown in Fig. 2, where the cost per unit capacity decreases as the capacity increases. An adequate approximation of the cost function of unit j with capacity x_j is obtained using the fixed-charge cost function given by:

$$C_j \, (y_j, x_j) = \alpha_j \, y_j + \beta_j \, x_j$$

$$x_j^L \, y_j \le x_j \le x_j^U \, y_j \quad , \quad y_j = 0,1 \qquad (3)$$

This fixed charge cost function reflects economies of scale since a fixed charge α_j for the investment of plant unit j is only incurred when the associated binary variable is set to I, or equivalently when the unit capacity is greater than zero in which case the variable cost term $J3_j x_j$ is activated. Furthermore, lower and upper bounds on the capacity of units (x^L_j and $x^\wedge_j$ can also be specified.

Therefore, the synthesis problem for a processing system can be transformed into a problem consisting of selecting values of the binary vectors y, y^d and the continuous vector x^c in the mixed- integer linear program (MILP):

$$\min \quad C = \{a/\ y \bullet (a/\ y^d \bullet (fi)^y\ x^c$$

$$\text{s.t. } E_1\ y^d \bullet E_2\ x^c = e$$

$$d^L \pounds D_1\ y \bullet D_2\ y^d \ll D_3\ x^c \pounds d^u$$

$$y_j = 0\ ,\ 1 \qquad j = 1,2,...n_y \tag{4}$$

$$y^d_j = 0\ ,\ 1 \qquad j = 1,2,...nJ$$

$$x^c \pounds 0$$

where C is the cost function, y, y^d , are binary vectors and x^c is the vector of continuous variables; a_1. a_2, *fi,* are cost vectors associated with the binary and continuous variables; e, d^L, d^u and E_1, E_2, D_1, D_2, D_3 are respectively vectors and matrices that define the constraint set of the problem.

It should be noted that in the actual implementation of this MILP model advantage can often be taken from the particular problem so as to reduce the number of binary variables, which can constitute a major bottleneck for obtaining efficiently the solution. Guidelines for accomplishing this goal are given in Papoulias and Grossmann(l983a). Basically the idea is that binary variables for discretized operating conditions can be used to represent the existence of units. Furthermore, by considering topological relationships of units in the superstructure a large number of these binary variables can be eliminated. Two cases of particular importance are the following:

1. Units i exist if and only if base unit j exists, which allows the replacement of binaries of unit i by the binaries of unit j.

2. Units i exist if base unit j exists, which allows the assignment of a single binary variable to units i.

By making use of these guidelines one can very often derive mixed-integer linear programs which have a modest number of binary variables and therefore can be solved with reasonable computational effort. In the following sections several examples will be presented in different application areas which illustrate the versatility and scope that mixed-integer linear programming can have in process synthesis.

Utility Systems

In order to illustrate the application of MILP in process synthesis, the problem of utility systems will be considered first. This synthesis problem consists in designing a system for supplying fixed demands of electricity, power for several process drivers, deaerated water, cooling water, and high, medium and low pressure steam. The objective in the design is to determine the configuration and operating conditions of a utility plant that satisfies the given set of demands at minimum investment and operating cost.

In the formulation of the synthesis problem of utility systems many alternative configurations can be considered systematically by including them in a superstructure such as the one that is presented in a simplified form in Fig. 3. In this superstucture there are three steam headers at high, medium and low pressure levels respectively. In each pressure level discrete steam pressures and temperatures can be considered, but obviously only one operating state must be selected in any level. Steam can be generated with either fired or waste heat boilers operating at pressures and temperatures consistent with the conditions in the steam headers. The available steam in each header can be used to provide a required steam demand, drive steam turbines operating in this level, or otherwise be transferred to the next lower level steam header with pressure reductors where water is added to match the steam quality.

There are three types of power generating devices considered: steam turbines, gas turbines and electric motors. The steam turbines can be either of the condensing or backpressure type, with the possibility of extractions in both cases. The gas turbines are of the simple open-cycle type, with air as the working medium. The hot gases exhausting the turbine section can be either used in a regenerator to preheat the compressed air before it enters the combustor of the gas turbine, or it can be integrated as preheated air for further combustion in fired boilers or as heating medium in waste heat boilers (Sawyer,l966). Electricity can be produced by any combination of steam and gas turbines connected with a common shaft on an electric generator. Power demands for drivers can therefore be satisfied with steam turbines, gas turbines or electric motors. In order to complete the superstructure auxiliary units have to be included. There is an optional vacuum condenser depending on whether there are any condensing steam turbines used. There is also a water treater for the make-up water, and a deaerator that treats the feedwater returning to the boilers and the required process (deaerated) water demand. The water returning to the boilers is raised to the required pressure with a feedwater pump, and can be preheated with an indirect contact feedwater heater that uses medium pressure steam.

Given the superstructure described above, the synthesis problem consists in determining the configuration of the utility plant, the values of the operating pressures and temperatures of the three levels of steam, the type and capacities of boilers, and all steam flowrates. Also, it is necessary to determine the assignment of turbines or electric motors to electricity and power demands, as well the type of turbine used for each demand.

Papoulias and Grossmann (1983a) have derived a MILP model for the superstructure described above using as criterion for optimization the minimization of the total annual cost of the system. By exploiting the topological relationships in the superstructure they only require binary variables for each possible state at the steam headers, and for each potential gas and steam turbines and electric motors in the superstructure. This MILP model has been applied to a test problem taken from Nishio et al.(!980). The problem is to synthesize an optimal utility system servicing a petroleum refinery of 200,000 BPSD capacity. The set of the refinery utility demands is given in Table I. As can be seen , there is a demand for electricity, 10 external power demands for drivers, 3 internal power demands for the utility system, and demands for medium and low pressure steam, and dearated and cooling water. Also there is import of medium and low pressure steam and condensate return. Three discrete operating conditions were considered for each, the high pressure (HP) steam header, and the medium pressure (MP) header, and one for the low pressure (LP) header.

There were two cases studied in the above example problem. In the first case electricity was produced using only steam turbine generators which is the same problem solved by Nishio et al.(!980), who employing heuristic rules discarded the use of gas turbines for generating electricity. In the second case the possibility of producing electricity also with a gas turbine generator was also included in the superstructure. The problem sizes were 44 binary variables, 253 continuous variables, 107 constraints for the first case, and 45 binary variables, 261 continuous variables, 115 constraints in the second case. The optimal solution for both cases was obtained in approximately 90 seconds of CPU time on a DEC-20 computer, using the branch and bound algorithm of the LINDO computer code (Schrage, 1981).

The optimal configuration obtained in the first case has an annual cost of 26.82 M$/year and is shown in Fig. 4. The optimal configuration represents a condensing Rankine power cycle, that produces electricity with a combination of HP and MP steam turbines connected to the electric generator with a common shaft. The HP steam turbine is a backpressure turbine exhausting to the MP steam header, and the MP steam turbine is a condensing turbine with an extraction to the LP steam header. Power demands no. 3, no. 4, no. 6, no. 7 and no. 14 are satisfied with MP steam turbines exhausting to the LP steam header, while electric motors are used for the remaining power demands. The operating condition with the higher pressure (P = 96.53 bar, T = 713 K) was selected for the HP steam header, while the MP steam header operates at the intermediate pressure (P = 17.24 bar, T = 600 K) that was considered.

In the second case, the optimal configuration has a total annual cost of 15.73 M$/year# which corresponds to a 41% reduction in the utility plant cost when compared to the previous case! The basic configuration is a binary cycle utility plant as shown in Fig. 5. The gas turbine cycle (1st cycle) produces most of the electricity required, while the exhaust hot gases are integrated in the main boiler to be used as preheated air and consequently reduce the fuel consumption in the boiler. Notice that the Rankine cycle (2nd cycle) does not require a condensing section since all steam turbines are backpressure turbines. The remaining electricity is generated with a HP steam turbine exhausting to the MP steam header. The same power demands as in the first case are satisfied with MP steam turbines and electric motors, but in this case there is a smaller load for the steam turbine driving the cooling water pump (no. 14), and the electric motors for the boiler feedwater pump and boiler draft (no. 12 and no.13). Note that there are two small reductors used between the steam headers in order to balance the steam flows in the utility plant. The only difference in the operating conditions of this utility system when compared with the optimal design obtained in the first case is that the operating conditions with intermediate pressure (P = 69 bar, T=66I K) is selected for the HP steam header. Finally, it is important to note that this optimal binary cycle plant has 37.4% less fuel consumption with respect to the above design that uses no gas turbine generator. This reduction is clearly due to the integration of the exhaust gases of the gas turbine with the boiler.

As shown with this example, the MILP approach can indeed determine with reasonable computational effort minimum cost solutions for utility systems. The fact that potentially promising alternatives can be embedded in the superstructure and that they need not be discarded with heuristics produced in the above example savings of 37.4% in fuel cost and 41% in total annual cost. It is important to note that the proposed approach optimizes simultaneously both the structure and operating conditions of arbitrary utility systems, which is a great improvement over previous methods reported in the literature (Nishio and Johnson, l979,Nishio et al, 1980, Petroulas and Reklaitis, 1981; Linnhoff et al, 1982). Another important feature of the above model is that due to its mathematical representation it can easily be added to a MILP synthesis model for total processing systems as will be shown later in this paper.

Heat Recovery Networks

The heat recovery network is one of the crucial components in a total processing system. The synthesis problem consists in integrating in a network of heat exchangers a set of hot and cold process streams with given heat capacity flowrates and inlet and target temperatures. A set of utilities (e.g. fuel, steam, cooling water) is assumed to be available in order to provide the auxiliary heating and cooling that is required. The objective in this synthesis problem is to develop a network that satisfies the stream specifications at minimum total annual cost.

Due to the large number of possible network configurations and to the nonlinearities involved in the investment cost function of the heat exchangers, the main approach that has emerged in the last years is to develop the following targets which simplify and reduce the size of this synthesis problem:

1. Minimum Utility Consumption. This is the most important target for an efficient heat exchanger network, since it corresponds to the maximum heat integration that can be attained in a feasible network for a fixed minimum temperature approach. Also, since the cost of utilities is commonly the dominant cost item, this objective allows the elimination of many network configurations which are inefficient and costly. The prediction of minimum utilities can be performed prior to developing the actual heat recovery network structure as has been shown by Hohmann (I97I) and Linnhoff and Flower (I978). This design objective can be further refined as the prediction of minimum utility cost, when a variety of hot and cold utilities are employed.

2. Minimum Number of Units. Another important objective is determining the minimum number of heat exchanger units that is required in the network. This objective attempts to minimize indirectly the investment cost of the network since the cost of each exchanger is assumed to be a concave function of the area. As noted by Hohmann (1971), the minimum number of units is usually one less than the total number of process streams and necessary utilities.

3. Modification of Pinch Points. A pinch point can be regarded as a bottleneck that prevents further heat integration in a network. An example of a pinch point is shown in Fig. 6, in which the composite hot and cold streams of a process are plotted in a temperature/enthalpy diagram. Note that the presence of the pinch point limits the maximum heat integration that is possible. Therefore, it is important to identify the location of pinch points prior to developing a network, in order to consider changes in the process that can eliminate or modify these bottlenecks so as to enhance heat integration as dicussed by Umeda et a!. (1979).

The first two design objectives have been used in previous methods for the synthesis of efficient heat exchanger networks: Linnhoff and and Hindmarsh (1983) in the pinch design method, and Cerda et al.(i983) and Cerda and Westerberg (1983) in a LP and MILP formulation that is based on the transportation problem. Papoulias and Grossmann (1983b) have used a similar approach as the latter authors, but they used instead formulations that are based on the transshipment problem which reduces considerably the size of the problem.

The basic idea in the transshipment model for the heat recovery problem is as follows. Heat can be regarded as a commodity that is shipped from from hot streams to cold streams through temperature intervals that account for thermodynamic constraints in the transfer of heat. In particular the second law of thermodynamics requires that heat flows only from higher to lower temperatures, and therefore these thermodynamic constraints have to be accounted in the network model. This can actually be done by partitioning the entire temperature range into temperature intervals according to rules proposed by Linnhoff and Flower (1978), Grimes et al.(l982), or Cerda et al. (1983). These partitioning procedures guarantee the feasible transfer of heat in each interval of the network, given a minimum temperature approach. In this way, as shown in Fig. 7, it can be considered that heat flows from hot streams to the corresponding temperature interval, and then to cold streams in the same interval with the heat residual going to the next lower temperature interval. Therefore, the transshipment model for the heat recovery network has the hot streams and heating utilities as sources, the temperature intervals as the intermediate nodes and the cold streams and cooling utilities as the destinations. The heat flow pattern for each temperature interval is shown in Fig. 8.

Using this representation, and by performing the appropriate heat balances at each intermediate node, Papoulias and Grossmann (1983b) have developed LP formulations for predicting the minimum utility cost for the cases of unrestricted and restricted matches. In the former case the number of rows in the LP is only equal to the number of temperature intervals, while the number of variables is one less than the number of utilities plus number of intervals. This implies for instance that for a problem involving 20 process streams, and 4 utility streams the size of the LP is of only 26 variables and 23 rows. It should also be noted that the location of pinch points can be predicted with these LP models as they are associated with zero-heat residuals at the optimal solution.

The MILP version of the transshipment model is used to determine the matches and heat loads that have to take place in the network to achieve the predicted minimum utility cost with minimum number of units. Binary variables are assigned to the potential matches and are used in the objective function to minimize the number of units. Weighting factors can be associated to the binaries so as to reflect discrete levels of priority to the matches. These priorities can be assigned on the basis of location of streams in the plant, control and safety purposes or on the basis of materials of construction. Although this MILP formulation does not provide directly the heat exchanger network configuration, its solution contains all the necessary information to derive the network by hand (which matches should take place and the amount of heat they must exchange).

It is also important to point out that the LP formulation can be extended easily when the flowrates of the streams are variable. This feature is particularly useful for the case of synthesis of total processing systems as will be shown in the example for total processing systems later in the paper.

To illustrate the application of the transshipment models described above, consider the I0SPI problem (Cerda, 1980), which has 5 hot and 5 cold process streams as shown in Table 2. The LP transshipment problem which consists of 11 rows and 12 variables predicts that cooling water is is the only utility required (l877kW) and that no pinch point occurs. In order to obtain the network structure requiring minimum number of units the MILP model for I0SPI is solved with unity weights for the binaries. This MILP model has 30 binary variables, I72 continuous variables and II9 constraints and was solved in less than 30 seconds using LINDO on a DEC-20 computer. The optimal solution corresponds to an unsplit network with 10 heat exchanger units as shown in Fig. 9.

To illustrate the application of weights for preferred matches in problem I0SPI, it was assumed that four different levels of priority were assigned to the 30 possible matches shown in Table 3. As can be seen the highest level of priority p=l, was assigned to the matches with cooling water because of the advantage of controlling directly the target temperatures of the hot streams. For the remaining matches it was assumed that the 10 process streams were located in three different sections of the plant. Therefore, the level of priority p=2 corresponds to matches that take place within each of the three sections in the plant, the level p=3 corresponds to the matches that take place between the adjacent sections, and the lowest level p=4 takes place between the two sections that are furthest apart. By using the weights shown in Table 3, (see Papoulias and Grossmann, I983b), the network that w&s obtained is shown in Fig. 10. Note that this network has 10 heat exchanger units and involves 3 matches with p=l, 5 matches with p=2, and one match for both p=3 and p=4 priority. Since the network of Fig.9 has 3 matches with p=l, 2 matches with p=2, 4 matches with p=3 and one match with p=4, it is clear that the network of Fig. 10 requires less integration among the three sections in the plant.

thus yielding a more useful network structure. The computer time requirements for this problem were considerably higher (9 min.) due to the existence of a large number of networks with minimum number of units. It should be noted that when the weights were set to one for simply obtaining a network with minimum number of units, the computer time was much smaller because the LINDO computer code would determine as the optimal solution the first network in the enumeration with 10 units.

Integrated Refrigeration Systems

A number of chemical processes have to operate at low temperatures requiring the use of expensive refrigeration systems. The synthesis of these systems can be regarded as an extension of the heat recovery network problem where the structure of the refrigeration system and heat recovery network must be determined simultaneously. Shelton and Grossmann (1983) have proposed a network model where a large number of alternative multistage structures can be embedded. These include the use of compressors, presaturators, economizers, intercoolers and exchangers for condensers, evaporators and intermediate loads.

The basic ideas in the network representation of Shelton and Grossmann (1983) are as follows: If a discrete set of temperatures is considered over the desired range and a box is drawn around each of these temperature levels, a simple network can be constructed that shows the flow of heat iji the refrigeration system. Fig. II shows the interactions of a single box, (B_j). Basically, these interactions are of two types: internal and external. Internal interactions, (L_{ij}) represent the passing of heat between temperature levels i and j within the refrigeration system. External interactions involve the passage of heat between the refrigeration system and the surroundings and are represented by H_j and C_j. The internal links in the network represent compressors operating between the specified temperature levels, while the remaining links represent either intermediate loads, (C_j) that add heat to the sytem or intercoolers, (H_j) that remove heat from the system. By assuming that the inlet to all compressors is saturated vapor, the work associated with each link can be shown to be independent on whether presaturators, economizers or indirect heat exchange is used at each refrigeration stage.

Since each box is associated to a given temperature level, it is clear that the box represents the connection between two successive stages in which the high temperature side of the lower stage passes heat to the low temperature side of the higher stage. Therefore, each box in the simple network can be partitioned into two nodes, *a* and *p* which represent the lower stage and the higher stage, respectively. A link (D_j) is included to represent the passage of heat between stages at level j. From Fig. 12, it can be seen that the intercooler, (H_j) is contained in the lower stage and the intermediate load (C_j) is contained in the higher stage. Based on these considerations, an individual box j can be restructured as shown in Fig. 12.

Two possible units can be used to pass heat between nodes *a* and *p.* These units are the economizer and presaturator. Depending on the amount of heat removed by the intercooler, the network structure can be associated to physical flowsheet structures that define the existence of presaturators or economizers. Finally, the heat effects of the hot and cold processing streams can be accounted for by merging them in a superhot and supercold stream through a "parallel" transshipment representation. The final network representation for integrated systems is shown in Fig. 13.

This network can be modelled as a LP for predicting a lower bound on the utility cost. This bound will underestimate the energy requirements since it will use all possible stages as no capital costs are included. However, a MILP formulation can be derived for the case when the objective is to find a structure that minimizes the total annual cost (investment and operating cost). In this case the binary variables are associated to the links that correspond to the comperssors. Since the number of the binaries can become rather large the combinatorial problem is reduced by limiting the maximum compression ratio and by disallowing nested cycles.

To illustrate the application of this network model, and to show the advantages of synthesizing simultaneously the heat recovery network with the refrigeration system, consider the problem given in Table 4 which involves one hot and one cold processing stream. A minimum temperature approach of 10K was assumed for the heat exchange, as well as a temperature change of 10K for each one of the potential stages in the refrigeration system. Refrigerant 22 was selected for this problem among various candidates on the basis of a performance index developed by Shelton and Grossmann (1983).

Two cases were considered for the solution of this problem. In the first one the process streams were integrated for maximum heat exchange, and then the refrigeration system was synthesized based on the resulting cooling duty. This decomposition scheme would be commonly used with the techniques that are currently available. In the second case the heat recovery network was synthesized simultaneously with the refrigeration system. In both cases the objective is to minimize the total annual cost for which the investment cost of the compressors and the utility costs (steam, cooling water and electricity) were considered. The problem size for the MILP in the former case is 9 binary variables, 80 continuous variables and 65 rows; the MILP for the latter case has 13 binary variables, 192 continuous variables, and 128 rows. Both MILP's were solved in less than 3 min. with the computer code LINDO (Schrage, 1981).

The optimal configuration for the first case has an annual cost of $38,500/yr and is shown in Fig. 14. Note that three stages are required in the system and that the cooling load of stream H1 is supplied by the two bottom stages. The optimal configuration for the second case is shown in Fig. 15 and has an annual cost of $27,600/yr. Thus, savings of the order of 28% are achieved for the case of simultaneous integration! Note that three stages are also required in this second case, but now stream C1 is split in such a way that it is integrated into the refrigeration system by exchanging heat with the outlet streams of the compressors in the two top stages. This has the effect of eliminating the use of cooling water and of lowering the temperature in the top stage down to 300K with which the work requirements are reduced from 4.64kW down to only 0.23kW. Furthermore, the steam requirements in the system are also reduced from 330kW down to 294kW.

This example then shows the importance of having a common mathematical framework that allows to synthesize simultaneously the heat recovery network together with the refrigeration system.

Total Processing Systems

In order to determine the optimal design of a total processing system, it is necessary to coordinate the synthesis activities for the three basic components of the system: chemical process, heat recovery network, utility system (see Fig.D.This coordination should enable the evaluation of different configurations of the chemical plant, as well as the heat recovery network and utility system, by taking explicitly into account the interactions. This can be accomplished if the synthesis of a total processing system is formulated as a MILP in which the three components are synthesized simultaneously. The following strategy has been proposed by Papoulias and Grossmann (1983c):

Step I. A superstructure is developed for the chemical plant which contains for instance different reactors or separation sequences that are to be analyzed. These alternatives would be postulated based on a preliminary screening by the design engineer (e.g.see Douglas,l982). The heating or cooling duties in this superstructure are treated as a set of hot and cold streams for the formulation of the heat recovery network in Step 2. The corresponding MILP for the chemical plant can be derived using the model proposed by Papoulias and Grossmann (1983c).

Step 2. Given all the hot and cold process streams in the superstructure of the chemical plant, the temperature intervals for the heat recovery network are derived based on their possible set of discrete inlet and outlet temperatures. With the temperature intervals, the transshipment model for minimum utility cost is formulated. In this model the flowrates of the process streams appear as variables that depend on the actual structure of the chemical plant. Since the LP transshipment model does not define explicitly the configuration with the exchangers of the heat recovery network, its investment cost is estimated as a linear function of the total heat transferred in the network. This clearly requires the assignment of a unit cost which in general provides only a rough approximation.

Step 3. The superstructure of the chemical plant together with the transshipment model for the heat recovery network will require different demands that have to be satisfied by the utility system. Therefore, a superstructure of the utility sytem and its MILP formulation can be derived as discussed previously in the paper. In this case, however, the demands for the utility system are not fixed parameters, but variables which depend on the structure of the chemical plant and the heat recovery network.

Step 4. The MILP models of the chemical plant and utility system, and the LP transshipment model for the heat recovery network are combined together so as to define a MILP model for the total processing system. This MILP model for the total processing system can then be solved with any standard branch and bound enumeration code so as to yield the optimal configuration of the chemical plant and utility system. In this way by simultaneously solving the resulting MILP problem, the total processing system can be synthesized by taking explicitly into account the interactions of the three major components. It should be noted that in general this will produce a different result than the case when the chemical plant is synthesized first, followed by the heat recovery network and lastly by the utility system.

Step 5. Having solved the MILP of the total processing system, the solution of the LP transshipment model will provide the minimum utility cost for the chosen chemical plant, since heating and cooling utilities provided by the ultility system incur in positive incremental costs. Since this solution will define the existing process and utility streams, the actual configuration of the heat recovery network with minimum number of units can be derived in this step with the MILP transshipment model.

The efficiency of this synthesis strategy is clearly dependent on the size of the resulting MILP model for a total processing system. However, the MILP model for utility systems and the LP transshipment model for heat recovery networks yield problems of reasonable size. Therefore, the MILP model for the total processing system can afiso be of reasonable size provided that only selected alternatives are included in the superstructure of the chemical plant.

In order to show the application of the synthesis strategy for total processing systems the following example from Papoulias and Grossmann (1983c) is considered. Assume that it is desired to manufacture 1000 tons/day of product D (liquid) using as feedstock a gas which contains chemicals A, B, C. The basic chemical reaction for this process is A+ B -> D + E, which is exothermic and produces the by-product E; chemical C is assumed to be an inert component. For this chemical plant, the basic steps of the process would first involve compression of the feed, next a recycle loop containing the reactor, flash unit, absorber, purge and compressor; the final step would involve a distillation sequence to obtain D as essentially pure component. It will be assumed here that the designer, having done a preliminary screening is faced with the following major choices in the process:

1. The reaction can be carried out with two different types of reactor at either high or medium pressure.

2. Since the solvent W must be added in the absorber, the components for distillation are D, E, W. Therefore the direct and indirect sequence of distillation are considered. In either of them the first column can operate at medium or at low pressure.

3. To avoid the build-up of inert C in the recycle loop, a purge rate must be selected, which in turn will have a major effect on the overall conversion of component A in the process.

Given these choices, the objective in the design problem would be to determine the configuration of the chemical plant, together with its heat exchanger network and utility system, in order to maximize the annual profit. This example will be solved with the above cited strategy and compared to the case when the three components are synthesized separately in order to illustrate the advantages with an integrated synthesis approach.

To apply the MILP strategy for total processing systems, the superstructure of the chemical plant is derived according to alternatives specified by the designer as shown jn Fig. 16. Note that the feed preparation step consists in compressing the feed to the required pressure of the reactor. Since the reactor can be selected at either the pressure of 40 bar or 100 bar, a single stage compressor or a two stage compressor with interstage cooling are embedded in the superstructure respectively. There are two reactor types, and for each a medium (40 bar) or high (100 bar) pressure can be selected. In both reactors higher conversions are obtained at the higher pressure. Because the conversions per pass in the reactors are low (10 and 18% for reactor Cl, 16 and 25% for reactor C2), the reactants are separated from the products and then recycled to the reactor so as to increase the overall conversion. Since components A, B and C of the reactor effluent are essentialy noncondensible, a flash is used to partially recover in the bottoms products D and E. The vapor from the flash enters an absorber where most of the remaining products D and E are absorbed by solvent W, and then mixed with the products recovered in the flash. The vapor stream exiting the absorber contains mainly the components A, B, C_r and part of this stream is purged in order to avoid build-up of inert component C in the reactor recycle loop. The values to be investigated for the purge rate are .5%, 2%, 5%, 10%. The rest of the vapor stream is recompressed and then mixed with the compressed feed to the reactor. For the product purification step, two possible sequences of distillation columns are considered for separating components D, E, and W. The first one is the direct sequence consisting of separation (D/E,W), where the most volatile component D is removed at the top, followed by separation (E/W) where at the top of the column by-product E is removed while solvent W at the bottom is recycled to the absorber. The indirect sequence consists of separation (D,E/W), where solvent W is drawn at the bottom to be recycled to the absorber, followed by separation (D/E) where product D is recovered at the top, and by-product E at the bottom of the column. For both sequences, the first separation column can operate at 20 bar or at 6 bar, whereas the second column operates at 5 bar.

In order to formulate the MILP synthesis model for the chemical plant, the linear equations and inequalities describing the performance of all plant units considered in the superstructure are derived. In this example problem this was done using shortcut methods for modelling the reactors, flash, absorber and distillation columns as outlined by Westerberg (1978). The heat recovery network corresponding to all process streams and utilities for this example is modeled using the transshipment model for minimum utility cost. The minimum temperature approach was taken as 10 K, and the heat exchanger investment cost was assumed to be $2 per kW of total heat transferred in the network. Finally, for the synthesis of the utility system supporting the chemical plant and heat recovery network, the MILP model discussed previously in the paper is employed. For the above example problem, it was assumed that 16,050 kW of electricity would have to be generated in addition to the power, heating and cooling demands required for the chemical plant and heat recovery network. The discrete operating conditions (pressures and temperatures) for the three steam headers, vacuum condenser and gas turbines exhaust, and the cost data were the same as the values considered in the example problem for utility systems. The integrated MILP for this example problem involved 34 binary variables, 269 continuous variables, 198 rows, and was solved using the branch and bound code LINDO in 3 minutes on a DEC-20 computer. The objective function for this formulation was to maximize the annual profit of the total system, and the value at the optimal solution was found to be 9.695M$/yr.

The optimal configuration and operating conditions for the chemical processing plant are shown in Fig. 17. Note that the feed passes through a two stage compressor with interstage cooling, and is compressed to 100 bars. The compressed feed is mixed with the recycle, and then enters the cheaper reactor Cl that has 18% conversion per pass. The reactor effluent is separated in a flash unit where part of the products D and E are recovered in the bottoms, while the vapor goes to the absorber that uses solvent W to recover most of the remaining products D and E. The optimal purge rate in the splitter is found to be 2% of the vapor stream exiting the absorber, with the remaining stream being recycled to the reactor after being recompressed. The optimal sequence of distillation columns necessary for product purification is the direct sequence at the lower pressure. The first column operates at 6 bar and separates the most volatile product D from components E and W that is recycled back to the absorber.

The hot and cold process streams are shown on the flowsheet of Fig. 17 with circles that indicate the type (H=hot, C=cold) and the number of the stream. The optimal transshipment network determined at the solution of the integrated MILP model gives the flowrates of all process streams and required utilities. The heat flows for this transshipment network are shown in Fig. 18. Note that the pinch point of the heat recovery network is located at 381 K - 371 K which ensures that minimum utilities are employed in the heat recovery network. The minimum heating utilities are 53.7 Ton/hr of MP steam and 242.4 Ton/hr of LP steam, and the minimum cooling is 6487 Ton/hr of cooling water. It is interesting to note that although two heating ultilities are selected at the optimal solution, there is only one pinch point in the network. The total amount of heat exchanged in this heat recovery network is 716 MegaWatts.

With the information obtained from the transshipment network (flowrates of process streams and utilities), the MILP transshipment model is used to determine the minimum number of heat exchanger units and the network layout. This MILP transshipment model involved 22 binary variables, 80 continuous variables, 87 rows, and was solved using LINDO in approximately 7 seconds on a DEC-20 computer. The minimum utility cost network having the least number of units (15 units) is shown in Fig. 19. Note that this network does not require any stream splitting and contains one cycle (HI-C2). Also note that the only heat integration that takes place in the two distillation columns is in the reboiler of the first column (C3) with the effluent of the reactor(HI).

The optimal configuration and operating conditions for the utility system are shown in Fig. 20. Note that this design represents a binary power cycle, where the primary cycle is a gas turbine generator exhausting the hot gases to the boiler of the noncondensing -Rankin secondary cycle to be used as preheated air. A medium pressure boiler generates steam at 17.2 bars and 600 K, and three backpressure turbines are employed to satisfy the power demands for the feed compressor (11,837 kW), the recycle recompressor (4369 kW) and the cooling water pump (1690 kW). The power demands for the boiler draft fan (1164 kW), feedwater pump (269 kW) and solvent recycle pump (26l kW) are provided with electric motors. Observe that both MP and LP steam are provided by the utility plant for the heating requirements in the heat recovery network. It is interesting to note that although the heat recovery network could use only LP steam, it is more efficient for the utility system to provide both MP and LP steam as it is then better balanced for satisfying the power demands.

In order to compare the integrated solution described above for the total processing system the problem was solved by decomposing it in the following manner. First the unintegrated chemical process was optimized separately by supplying heating, cooling and power utilities at nominal prices. With the resulting flowrates and temperatures of the hot and cold streams the heat recovery network was synthesized with the transshipment model. Finally, the utility system was synthesized for the power and steam demands obtained in the two previous steps.

Not unexpectedly, a different solution was obtained through this decomposition scheme. The annual profit for this case was 8.833 M$/yr, which represents a decrease of almost 9% with respect to the optimal integrated solution. It is interesting to note that the chemical process of the decomposed solution was actually not too different. It operated also at 100 bar, it had the same separation sequence, but it selected the more expensive reactor C2 (25% conversion per pass) and the higher purge rate of 5%. As a matter of fact this flowsheet was more energy efficient since its fuel consumption (22.59 ton/hr) for utility requirements were 4.4% lower. However, this flowsheet was more inefficient in the raw material utilization since it had an overall conversion of 85.3% which is 4.5% lower than the 89.8% conversion of the flowsheet of the integrated solution. Since raw materials and not energy was the dominant cost item, this explains why the optimal solution shown in Fig. 17 was obtained. This example then clearly shows the pitfalls associated with common decomposition schemes for process synthesis, and that energy may not always be the primary consideration for the optimal solution.

It is interesting to note that if the chemical plant and the heat recovery network are synthesized simultaneously with nominal prices for utilities, and the utility system is synthesized in a second step, Papoulias and Grossmann (1983c) found that in this example the solution is very similar to the one obtained with the integrated approach. The main difference was in the utility system which was forced to produce only low pressure steam.

A point that should also be apparent from this example is that the MILP aproach for total processing systems has great potential as a systematic tool for screening many alternative flowsheets. This should be particularly relevant in practice, where very often alternatives that are potentially attractive cannot be explored due to time limitations in a project. If this approach were to be implemented in a computer-aid that would automatically generate the MILP models, it would be possible at the initial stages of the project to direct the design engineers to the most promising alternatives which could then be analyzed in detail. It should be noted that the branch and bound codes that use depth-first enumeration will usually generate several feasible solutions before finding the optimal answer. Therefore, if these intermediate solutions are close to the optimal they could also be considered for a detailed analysis. Another way to generate several promising solutions different from the optimal, is to resolve the MILP to find solutions whose objective function value lies within a tolerance of the optimal solution.

Other applications with MILP

The previous sections have presented several applications of process synthesis with MILP techniques. However, it is important to point out that few other applications have also been recently reported. For instance, Andrecovich (1983) has formulated the synthesis of multi-effect distillation columns with heat integration as an MILP problem. He has proposed a procedure for generating a superstructure in which binary variables are associated to each potential column and where the heat integration problem is treated through the transshipment or transportation model. Papoulias and Grossmann (1983d) have considered the synthesis of flexible utility systems that must satisfy time-varying demands as a multiperiod MILP problem. This clearly shows the versatility that can be achieved when modelling synthesis problems through MILP techniques.

Although the clear advantage in the use of MILP is that efficient computer codes are widely available, it is also clear that it would be desirable to handle explicitly nonlinearities that are due to operating conditions such as pressures, temperature, reactor conversions and split fractions, rather than having to discretize these conditions at few selected points. The capability of handling nonlinearities would on the one expand the scope of synthesis problems that could be solved, and on the other hand it would avoid the problem of introducing extra binary variables in MILP models to treat variables that give rise to nonlinearities. The next section discusses briefly some of the options that are currently available for solving mixed-integer nonlinear programming problems, and a promising approach is outlined which could simplify the solution of these problems.

Mixed-integer nonlinear programming

The two major methods for solving MINLP problems are the branch and bound procedure and Generalized Benders decomposition method. In the branch and bound procedure (Garfinkel and Nemhauser, 1972; Balas, 1979), the basic idea is to perform a search in a tree where each node defines a partial assignment of the 0-1 variables. In this way each node gives rise to a nonlinear programming (NLP) problem in which some of the binary variables of problem (I) have fixed values, and the remaining ones are treated as continuous variables that are bounded between 0 and I. The branch and bound strategy enables one to enumerate only a subset of the total number of nodes in the tree in order to find the optimal solution. However, the number of nodes to be enumerated can be rather substantial if the size of the tree is very large as is commonly the case in synthesis problems. Therefore, since each node involves the solution of a large scale NLP, the computational requirements for this method are usually expensive.

The Generalized Benders decomposition technique (Benders, 1962; Geoffrion, 1972) requires the alternate solution of a NLP problem and of a pseudo-integer programming problem. The NLP problem arises from a fixed choice of all the binary variables. The pseudo-integer problem corresponds to the master problem where the binary variables are selected for the solution of the NLP problem in the following iteration. This master problem uses cutting planes derived from duality theory and provides a lower bound to the solution of the MINLP. The main drawback in Generalized Benders method is that · the number of iterations that are required to find the optimal solution is usually large. The reason is simply that in order to accumulate enough information through the cutting planes of the master problem and in order to restrict effectively the choices of the binary variables, one often has to solve a substantial number of NLP subproblems.

Recently, Duran and Grossmann (1983a) have proposed an algorithm which in a way is similar to Generalized Benders decomposition in that it solves a sequence of NLP and master problems. Firstly, they assume that the MINLP problem (1) has the special structure that the binary variables are linear and separable from the continuous variables which appear in nonlinear functions. That is, the problem has the general form

$$
\begin{array}{c}
\min \quad c^T \; y \bullet f \; (x) \\
\text{s.t. } h \; (x) = 0 \\
A \; y \bullet g \; (x) \; £ \; 0 \\
x \, 6 \, R^n \quad , \quad y£ \;\; \{O,1\}"\backslash
\end{array}
\qquad (5)
$$

which allows the modelling of a large class of synthesis problems.

The crucial difference in the algorithm of Duran and Grossmann (I983a) with respect to Benders decomposition is that the master problem is given by an MILP problem which performs outer-approximations on the feasible region of the superstructure by using primal rather than dual information from the NLP problem. Furthermore, this NLP is usually of much smaller size than problem (1) since with a fixed choice of the 0-1 variables many constraints and variables in the superstructure are trivially satisfied. The outer- approximations are obtained through function linearizations or by the use of linear underestimators. The advantage of this master problem is that it provides a better global approximation to the MINLP when compared to the pseudo-integer master problem of Benders. In fact, Duran and Grossmann (1983b) have proved that the lower bound of their master problem is always greater or equal than the lower bound predicted by Benders method. In this way the number of iterations required in solving successively the NLP and master problems can be greatly reduced. This has been confirmed in a test problem involving 8 binary variables, 9 continuous variables and 23 inequality constraints. The proposed algorithm required one-fifth of the CPU-time of the branch and bound method and one" half of the CPU-time of Generalized Benders decomposition.

Details of the algorithm are given in Duran and Grossmann (1983a), but Fig. 21 presents the basic steps in the context of process synthesis problems. First, a choice is made on the binary variables that defines a particular flowsheet. This flowsheet is then optimized for the continuous variables (reduced NLP problem). This solution then provides an outer-approximation of the superstructure which is used to construct the master problem (A-MILP). If no solution exists for this master problem the optimal solution is the current best flowsheet. If on the other hand the master problem has a feasible solution it will provide a new combination of binary variables that define a new flowsheet whose lower bound lies below the current best estimate. The cycle of iterations is repeated until no feasible solution is found in the master problem. Since the lower bound of the master problem increases monotonically as iterations proceed, this method can be regarded qualitatively as a "learning" method which will narrow down the options for flowsheet structures rather quickly as iterations proceed. Work is currently under way to test this algorithm with a chemical process together with the problem of heat integration in which variable flows and temperatures of process streams can be handled.

Discussion

This paper has emphasized not only general ideas related to algorithmic methods, but actual results of example problems that have been obtained with mixed-integer programming techniques. The primary motivation for doing this has been to show that mixed-integer programming can indeed be a useful tool in process synthesis. That it can greatly help the design engineer in making decisions for synthesis should be clear from the example problems where heuristic rules or simple decomposition schemes were shown to fail in finding lower cost solutions. Furthermore, the examples have also shown that by proper formulation of synthesis problems and by exploiting their structure, the computational expense with MILP techniques can be quite reasonable and certainly not prohibitive as it is sometimes claimed.

Finally, we are not suggesting to equate process synthesis with mixed-integer programming, nor are we suggesting that this approach should be used to remove engineers from the decision making process. It is clear that heuristics and thermodynamic targets are essential in making synthesis problems manageable, and that the design engineer should play a central role in this type of activity. However, it would seem to be unnecessary to restrict engineers to only manual trial and error methods when efficient algorithmic tools can aid them significantly in the search for better solutions.

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Table 1: Utility Demands and Imports for Example Problem

DEMANDS		
STEAM		
M.P. steam	125.1	Ton/hr
L.P. steam	187.3	Ton/hr
ELECTRICITY		
no. 1	32030	kW
EXTERNAL PCWER		
no. 2	818	kW
no. 3	1965	kW
no." 4	2020	kW
no. 5	1530	kW
no. 6	1940	kW
no. 7	3120	kW
no. 8	85	kW
no. 9	440	kW
no.10	203	kW
no. 11	650	kW
INTERNAL PCWER		
no. 12 (BFW pump)	to be calculated	
no. 13 (boiler draft fan)	to be calculated	
no. 14 (cooling water pump)	to be calculated	
WATER		
deaerated water	275	Ton/hr
cooling water	7306	Ton/hr
IMPORTS		
STEAM & CONDENSATE		
M.P. steam	224.0	Ton/hr
L.P. steam	50.2	Ton/hr
condensate return	120.1	Ton/hr

Table 2. Stream data of 10SP1 problem.

Streams	Fc_p (KW/°C)	T*(°C)	I* (°O	Q (KW)
Cl (Cold)	7.62	60	160	+762
C2 (Cold)	6.08	116	222	+644
C3 (Cold)	8.44	38	221	+1545
C4 (Cold)	17.28	82	177	+1642
C5 (Cold)	13.90	93	205	+1557
H6 (Hot)	8.79	160	93	-589
H7 (Hot)	10.55	249	138	-1170*
H8 (Hot)	14.77	227	66	-2378
H9 (Hot)	12.56	271	149	-1532
H10 (Hot)	17.73	199	66	-2358
W (Water)	42.66	38	82	1877

Table 3, Preferred matches for 10SP1 problem.

	Cl C2	C3	C4 C5	CW
H6	4	3	2	1
H7				
H8	3	2	3	
B9	2	3	4	
H10				

Level of priority	Weights
p - 1	6.25
p - 2	6.5
P - 3	6.75
p - 4	7

Table 4. Data for Refrigeration System

Stream	Flowrate (kW/K)	Supply Temperature (K)	Target Temperature (K)
Cl	4	270	370
HI	1	350	250

Cost of utilities:

Cooling water (300K) = $15.97/kW yr
Steam (440K) = $50.91/kW yr
Electricity = $608.33/kW yr

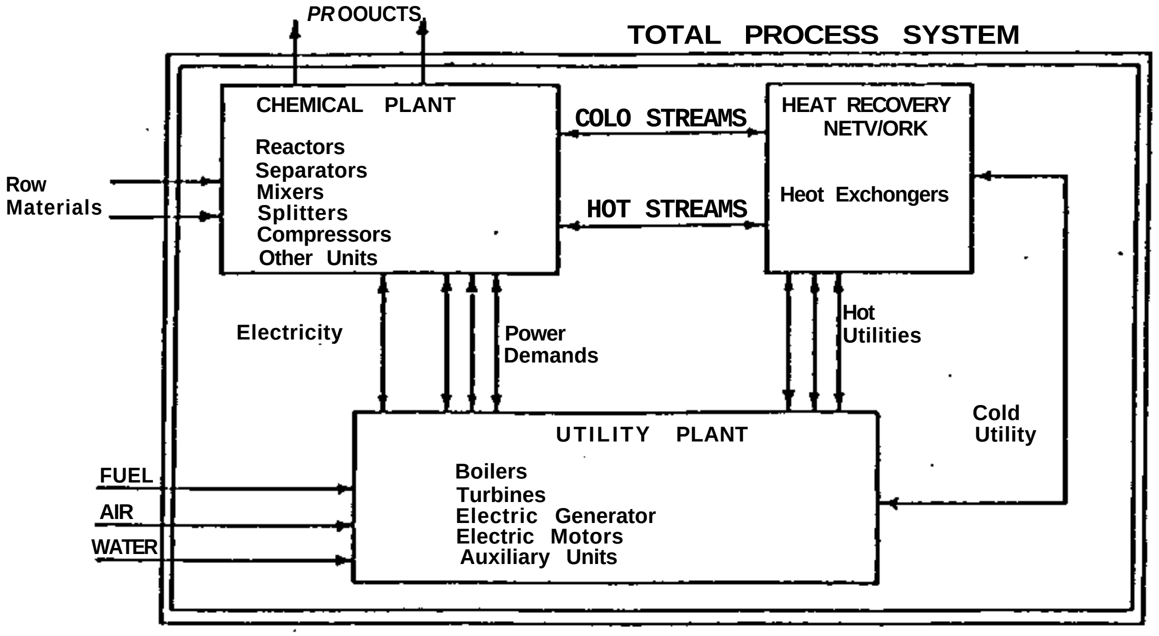
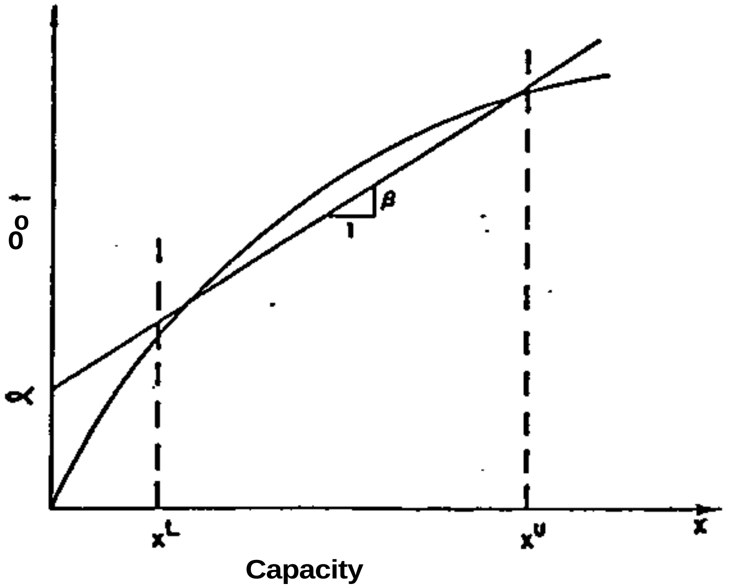


Fig. 1 Total processing system



Fig, 2 Approximation of concave cost function with fixed-charge cost function.

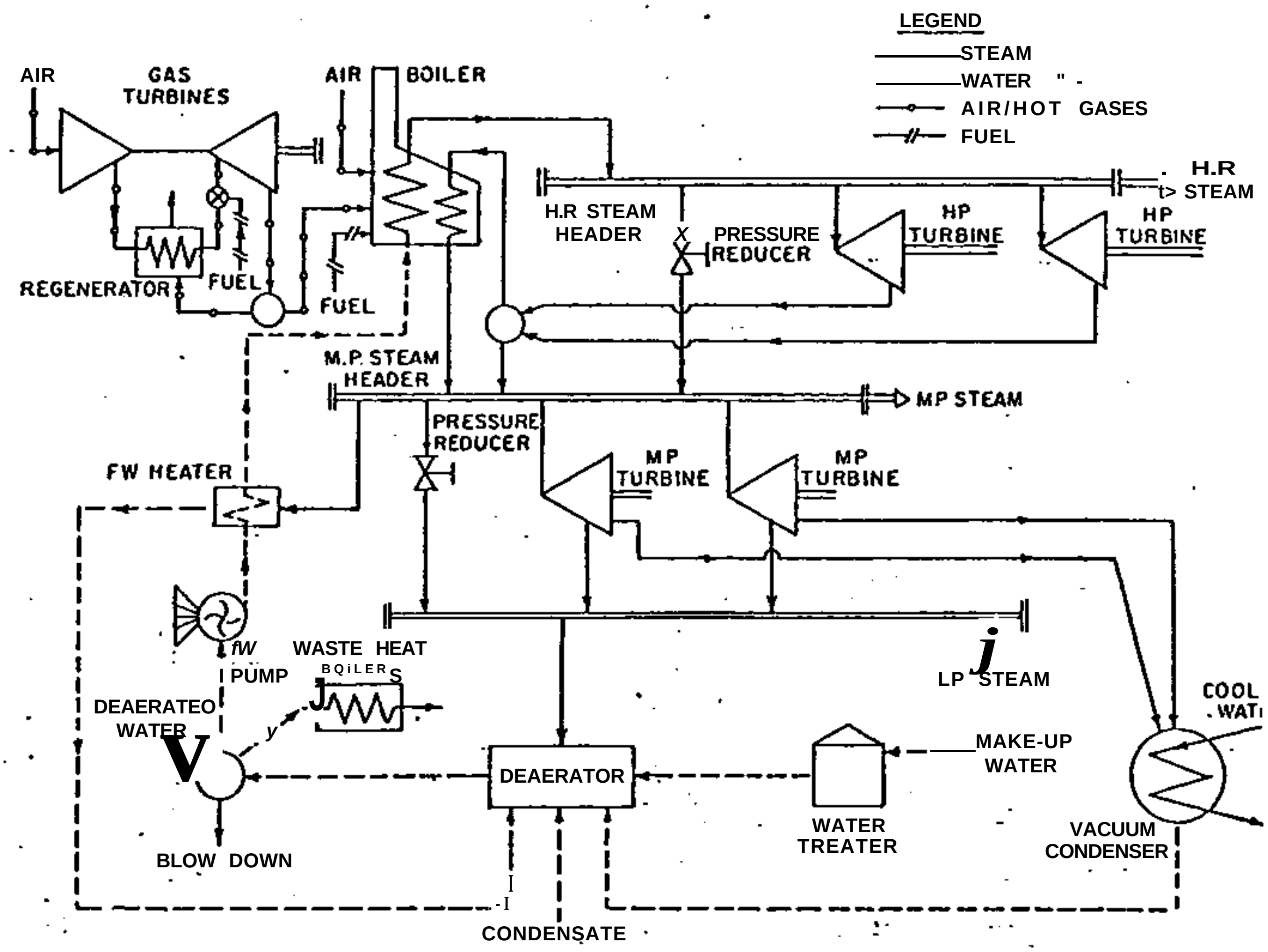


Fig. 3. Superstructure for utility system

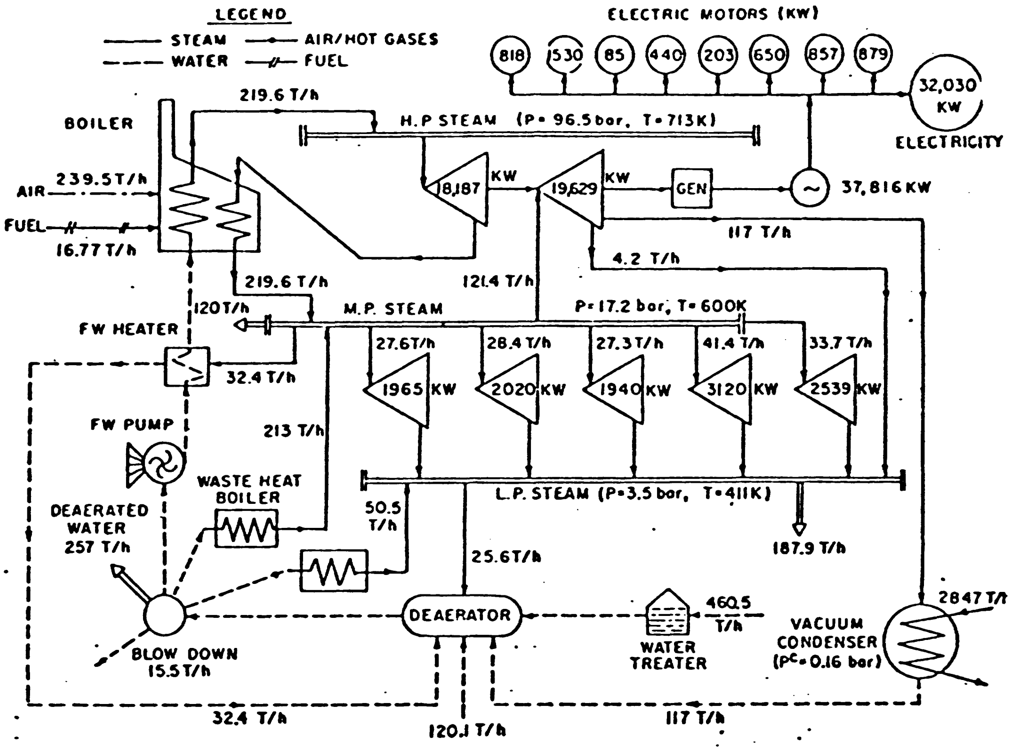


Fig. 4. Optimal solution without gas turbine generator

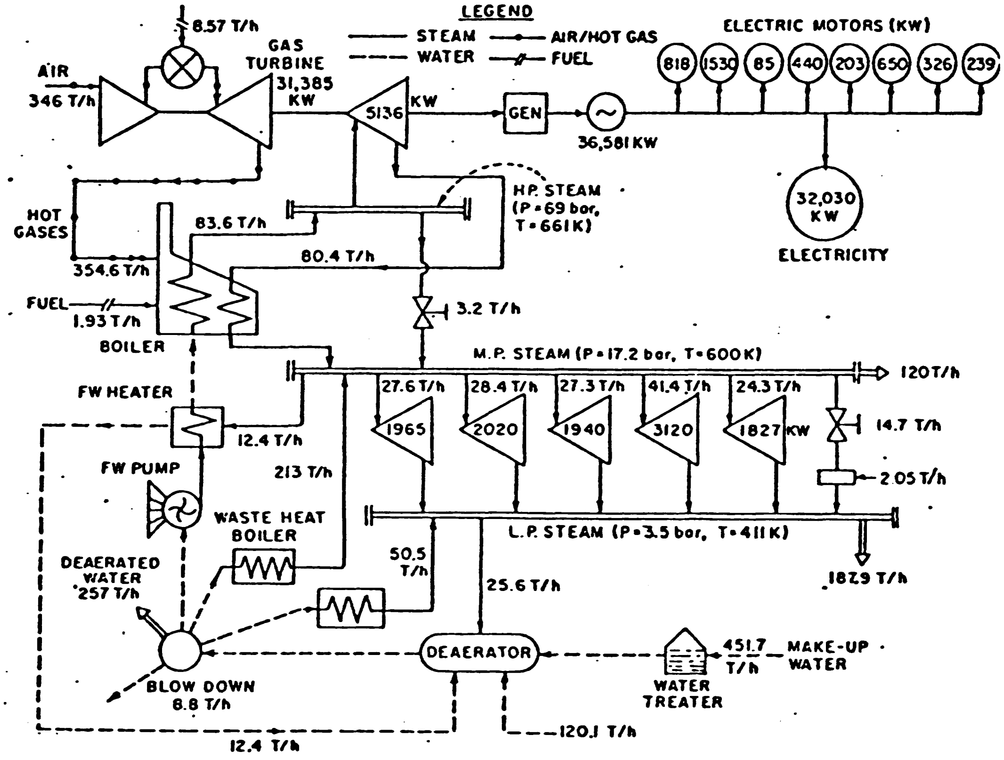


Fig. 5. Optimal solution with gas turbine generator

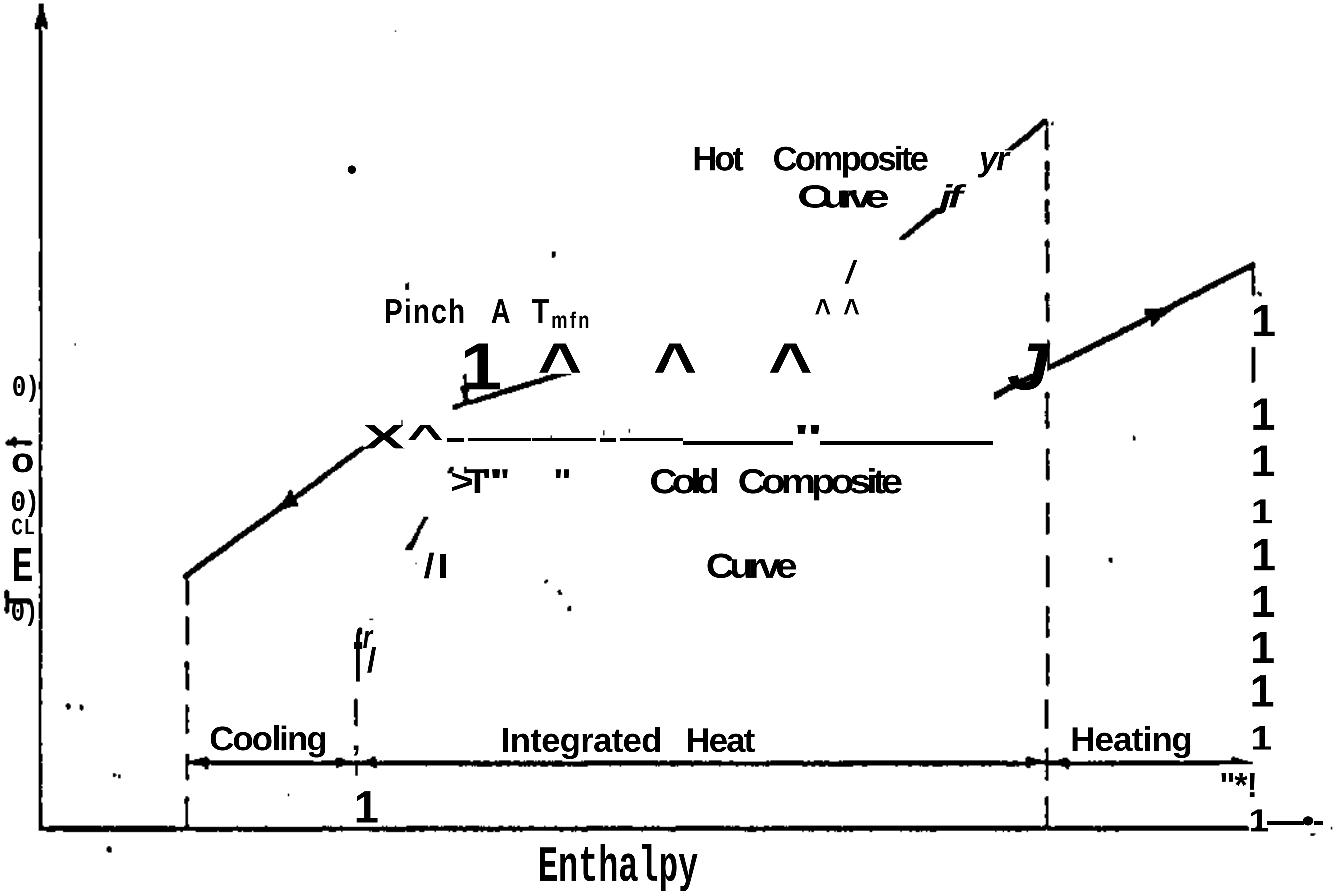


Fig. 6. Composite hot and cold streams for maximum heat integration

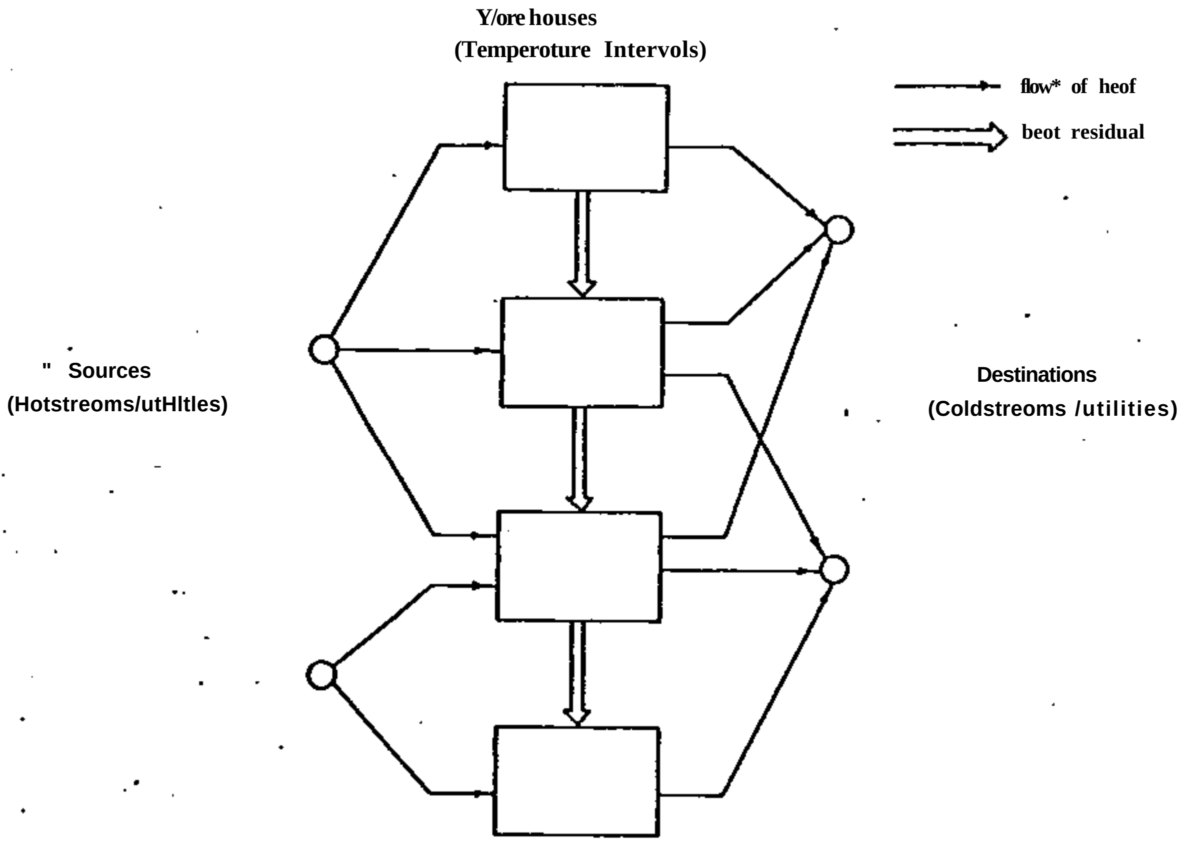


Fig. 7. Transshipment model for heat recovery network

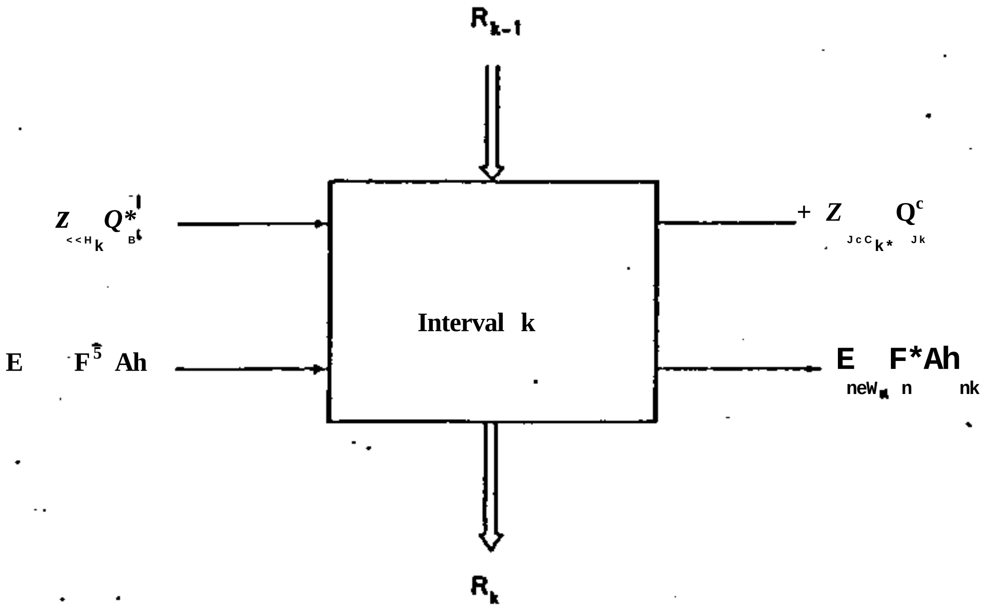


Fig. 8. Heat flow pattern in temperature interval k.

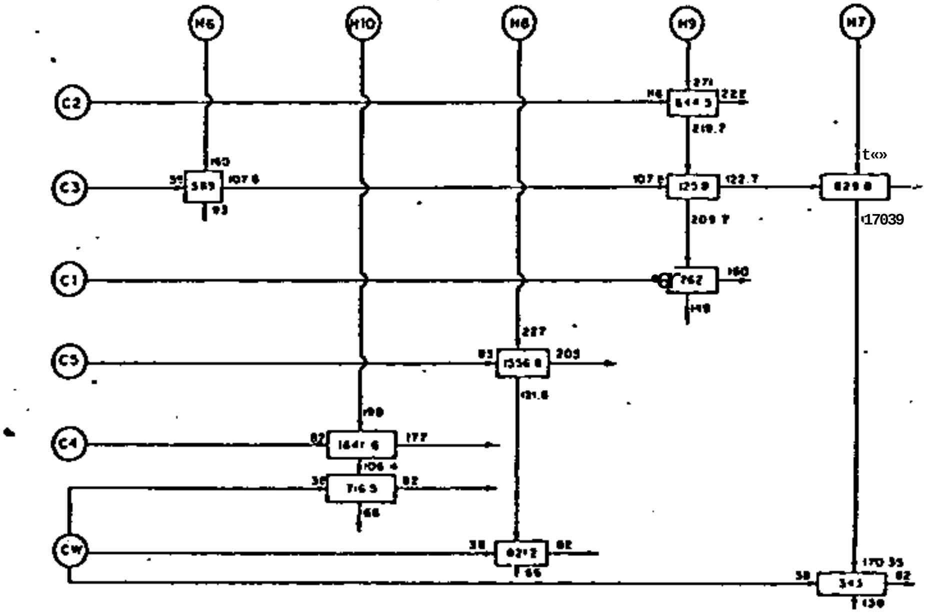


Fig. 9. Optimal network with no preferred matches.

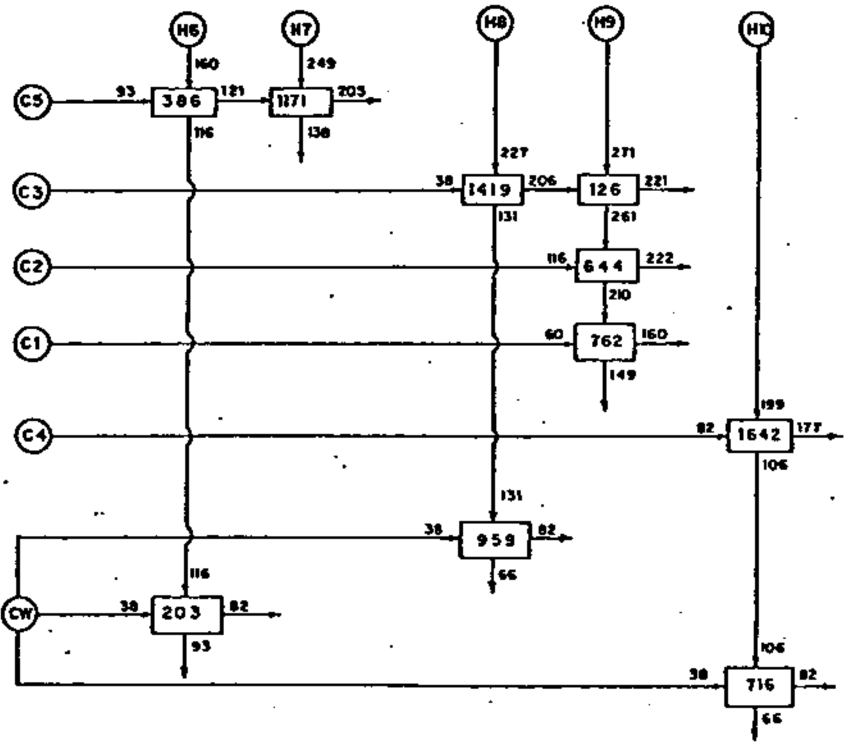


Fig. 10. Optimal network with preferred matches.

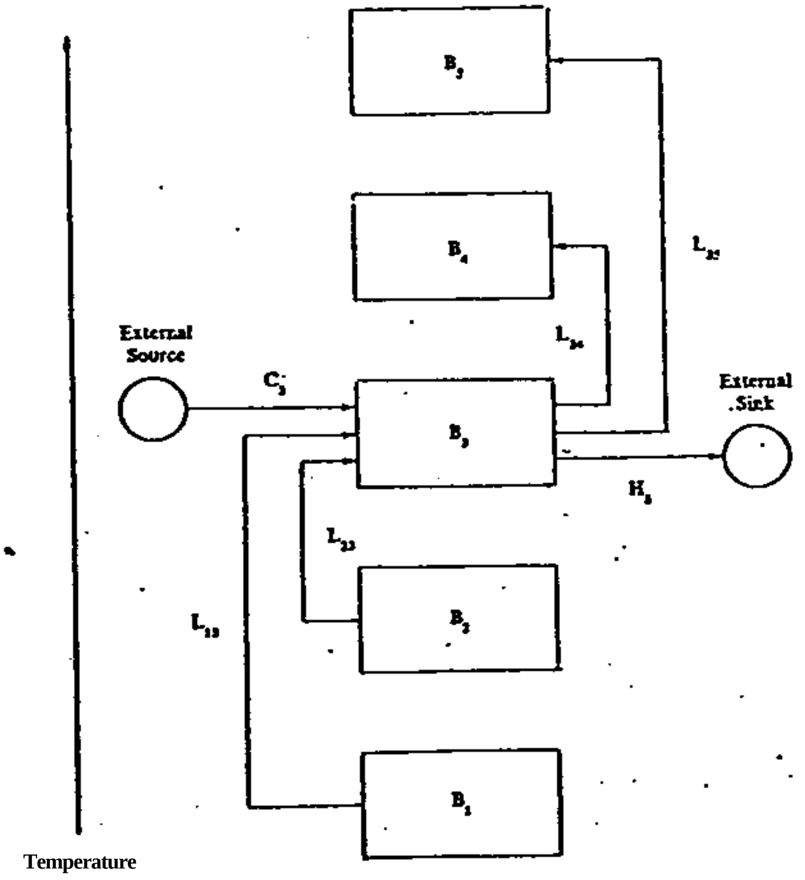


Fig. 11. Simple network representation for multi-stage refrigeration

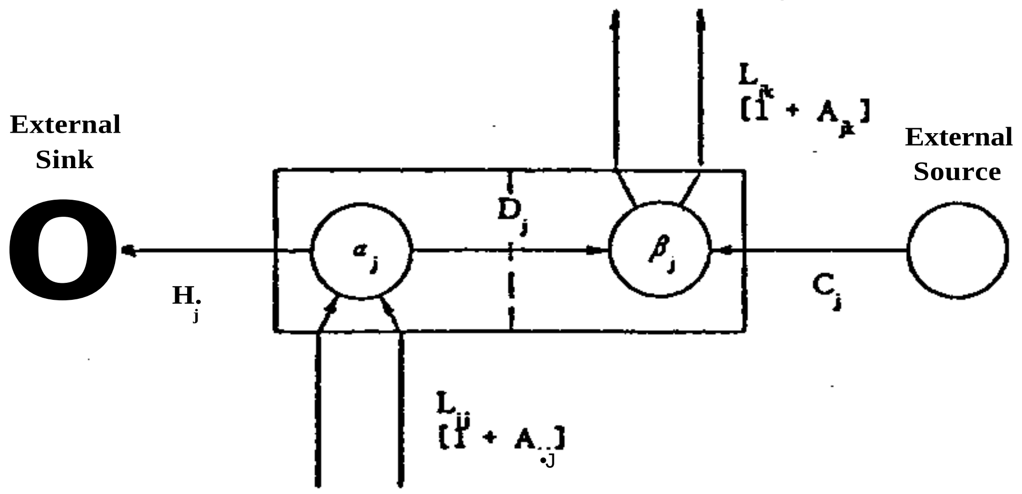


Fig. 12. Splitting of nodes in each individual box.

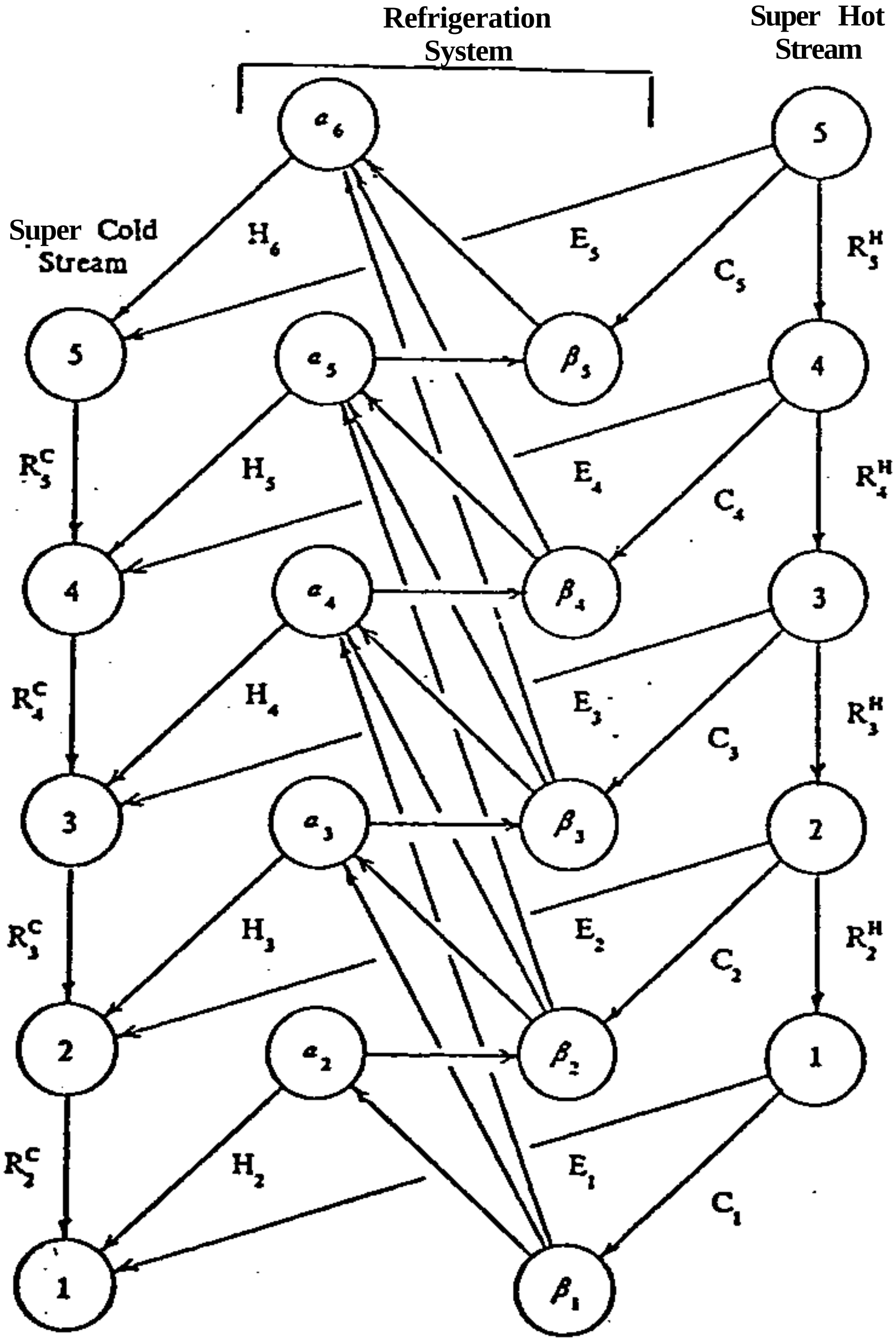


Fig. 13. Network model for integrated refrigeration systems.

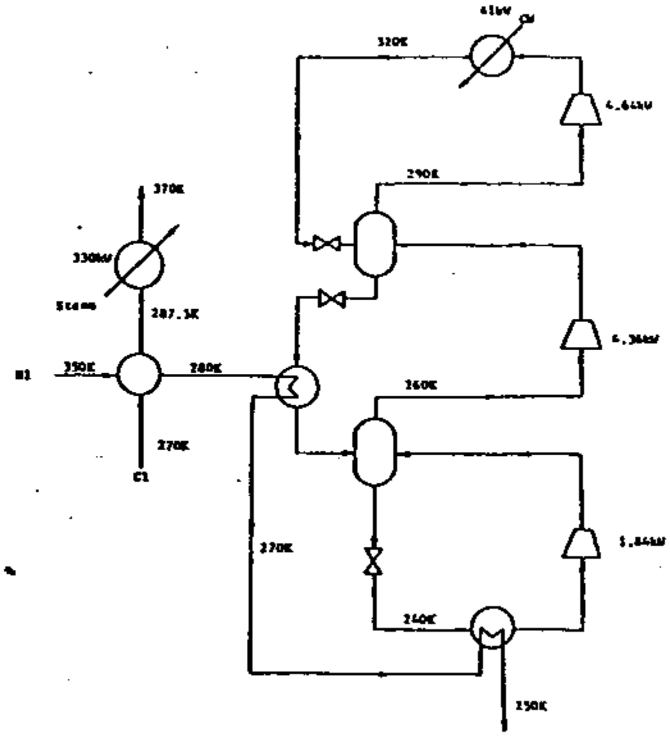


Fig. 14. Optimal configuration with sequential synthesis„

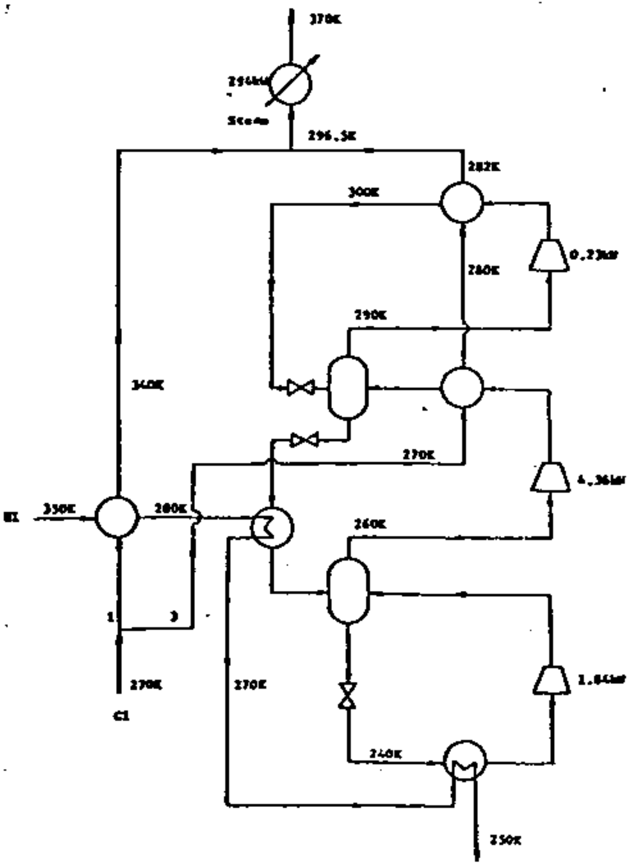


Fig* 15. Optimal configuration with simultaneous synthesis„

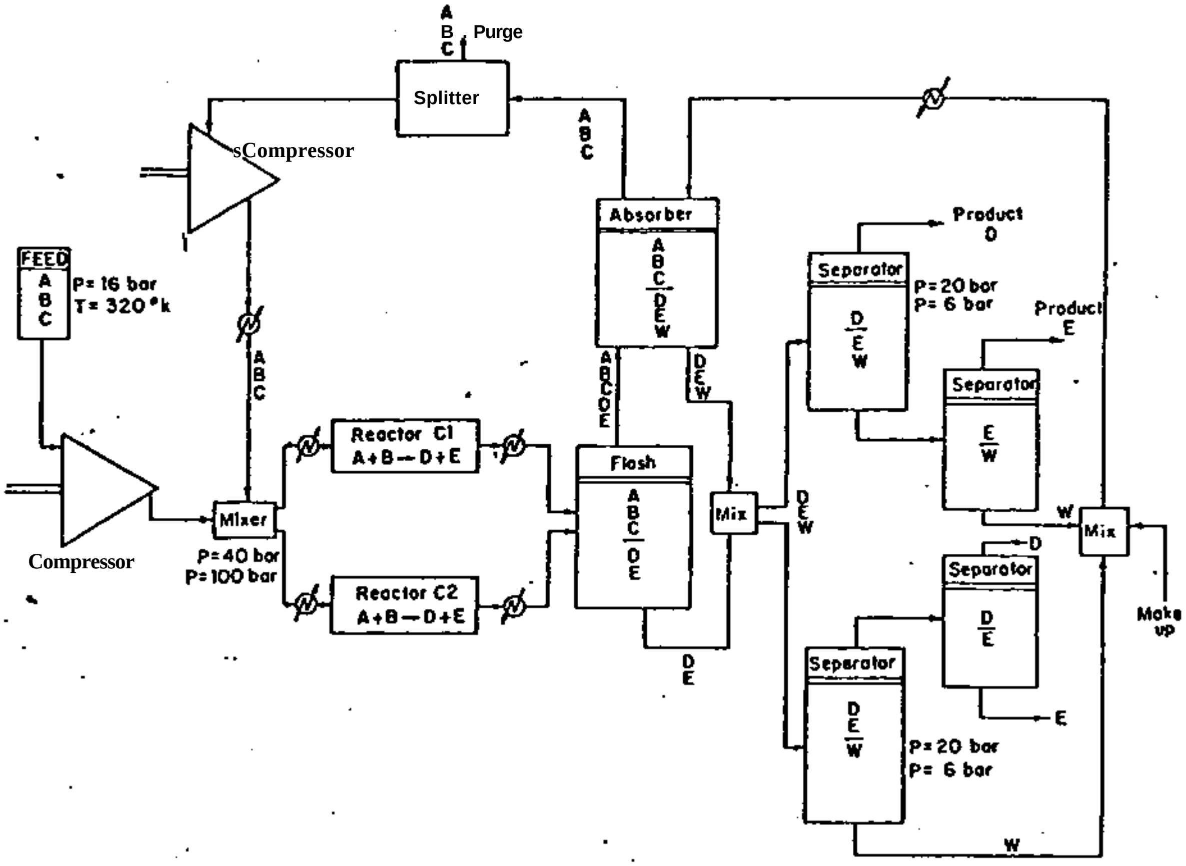


Fig. 16. Superstructure for chemical plant in total processing system.

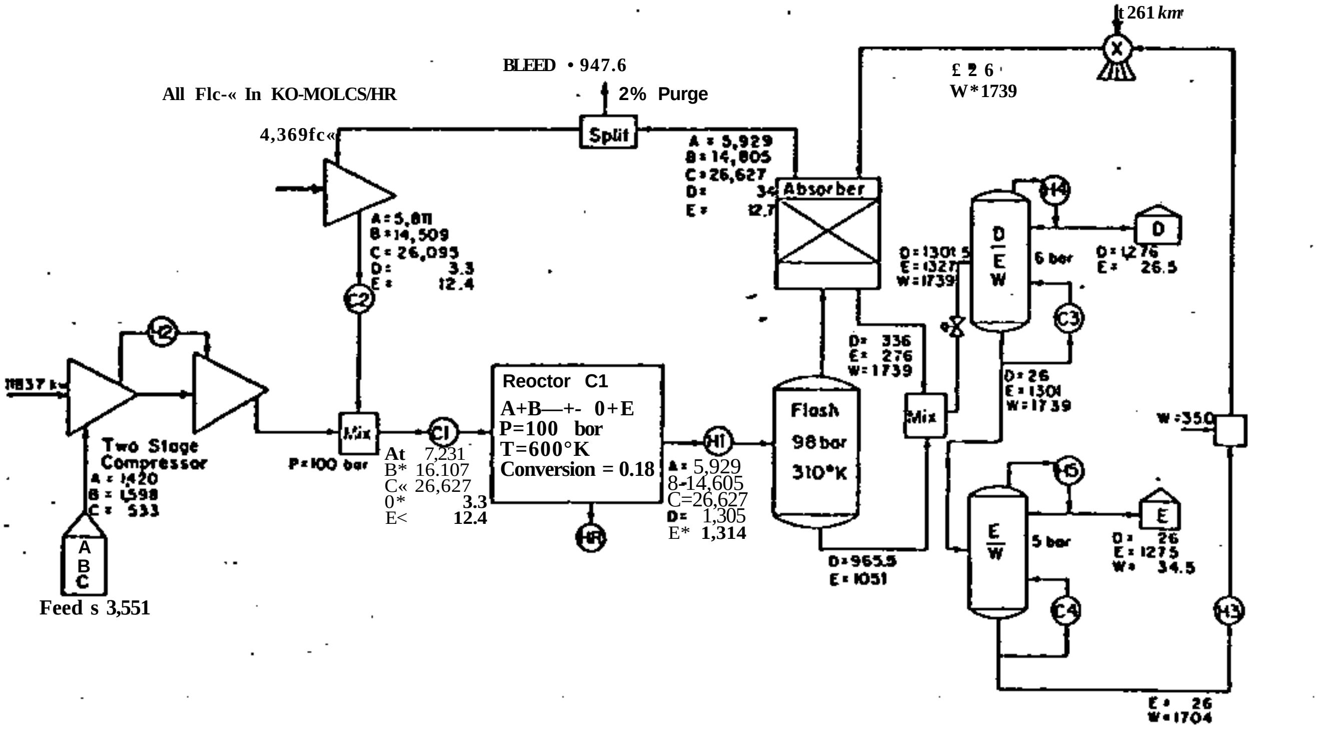


Fig. 17. Optimal configuration of chemical plant.

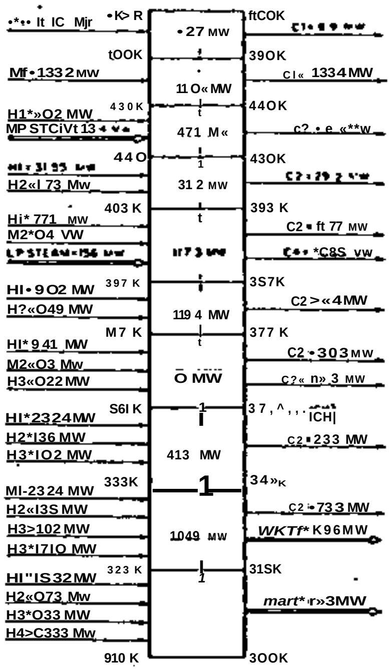


Fig. 18. Optimal solution of transshipment model.

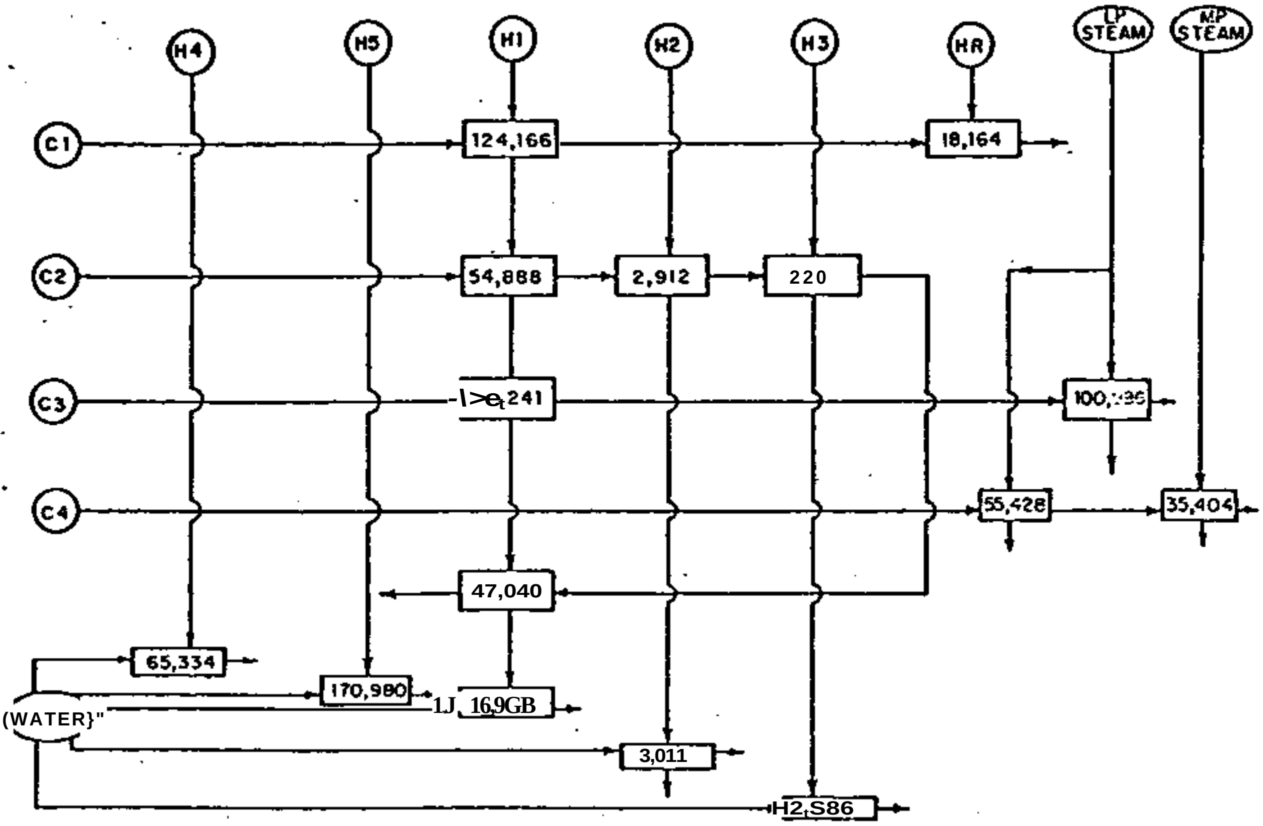


Fig. 19. Optimal heat recovery network.

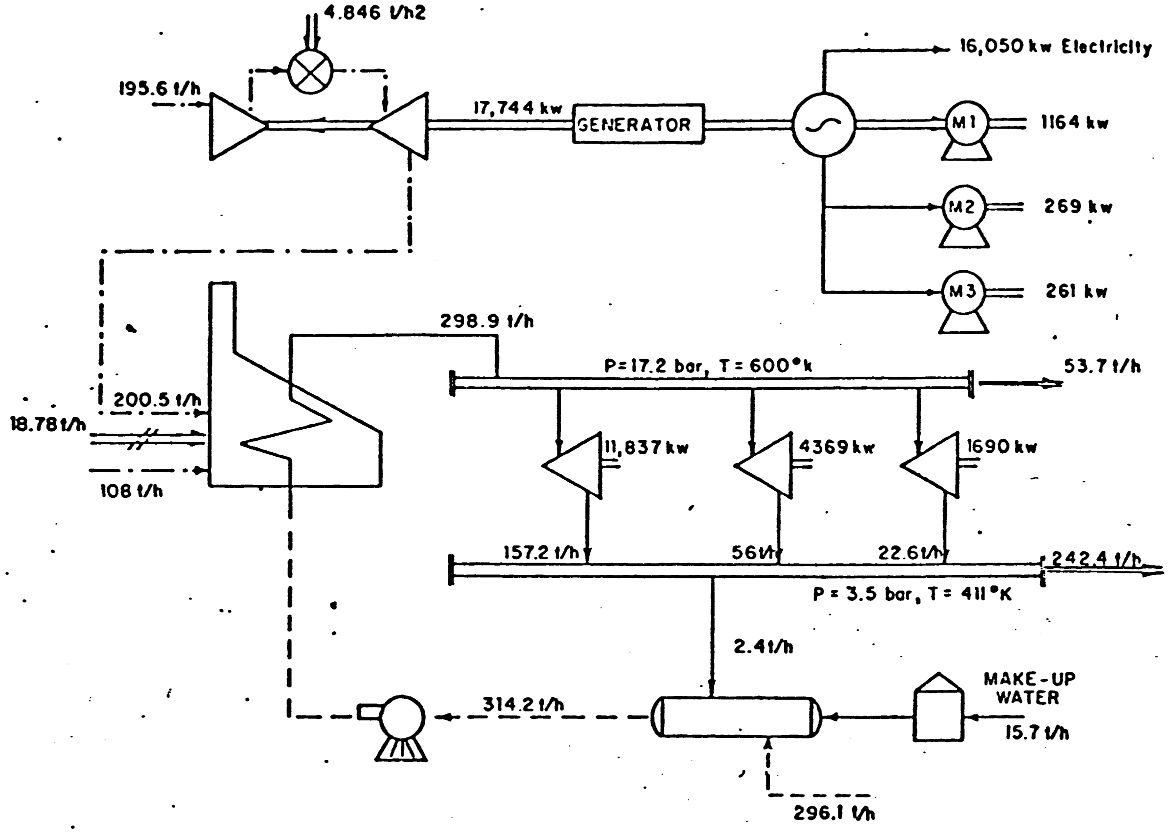


Fig. 20. Optimal configuration of utility system.

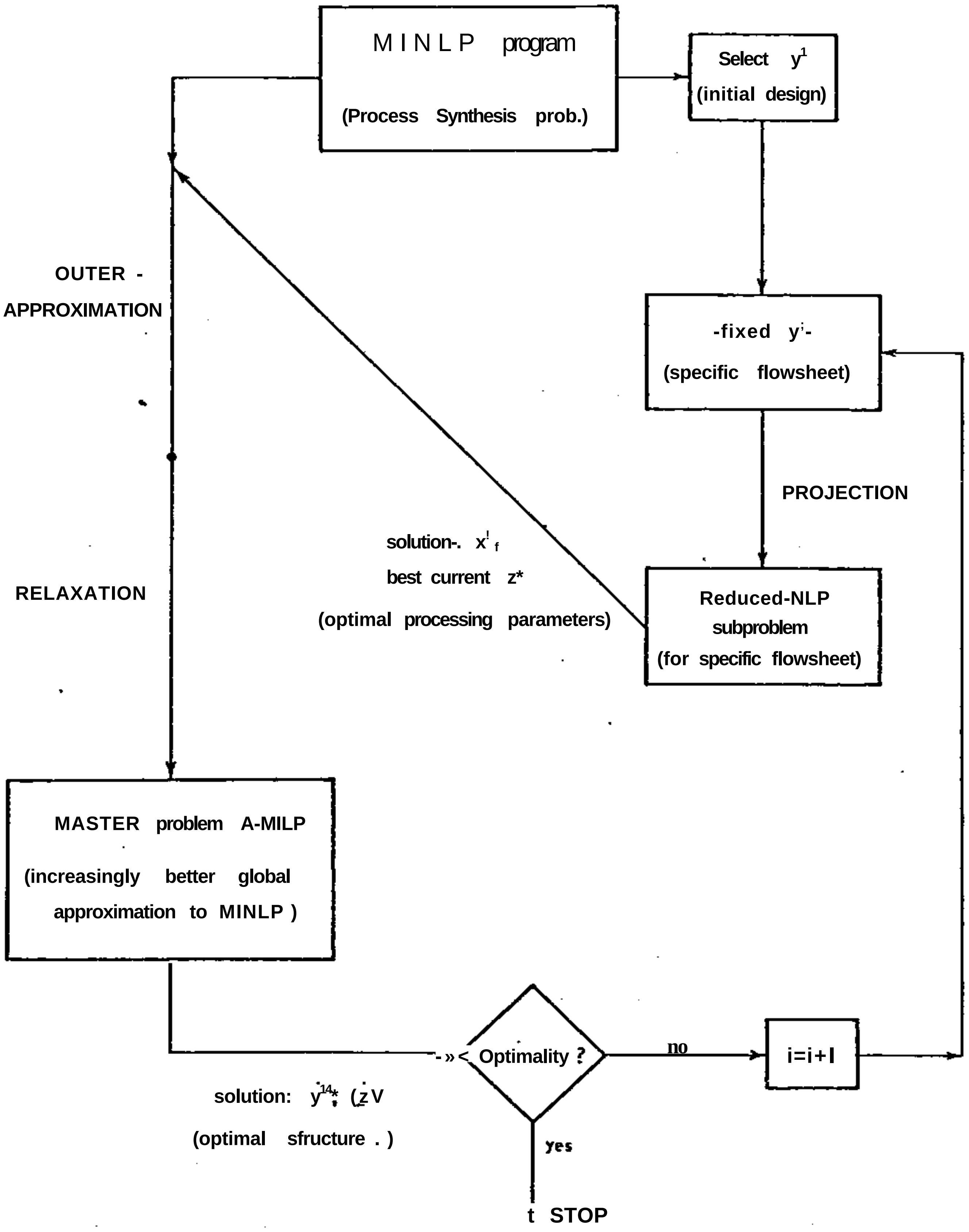


Fig. 21. Basic steps in outer-approximation algorithm for MINLP problem.