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\ STRUCTURAL OPTIMIZATION APPROACH IN PROCESS SYNTHESIS  
PART I: UTILITY SYSTEMS

by

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A STRUCTURAL OPTIMIZATION APPROACH IN  
PROCESS SYNTHESIS. PART I: UTILITY SYSTEMS

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## Abstract

A mixed-integer linear programming approach is presented for performing structural and parameter optimization in the synthesis of processing systems. This approach is applied to the synthesis of utility systems that have to provide fixed demands of electricity, power for drivers and steam at various pressure levels. A superstructure that has embedded many potential configurations of utility systems is proposed, as well as its corresponding mixed-integer programming model. The application of the model is illustrated with a large example problem.

## Scope

Process synthesis has been a very active area of research over the last fifteen years. Extensive reviews on the large number of publications in this area can be found in Hendry et al. [5], Hlavacek [6], Westerberg [18], Stephanopoulos [16] and Nishida et al. [7]. The basic approaches that have been suggested in process synthesis are the use of heuristics, thermodynamic targets and optimization techniques. In recent years there has been considerable skepticism on the usefulness of the latter approach (e.g. see [16]), the main arguments being that optimization techniques are inefficient for synthesis problems, and do not contribute to their physical understanding. Although there is no question that heuristics and thermodynamic targets have led to considerable progress in several types of synthesis problems (mainly heat recovery networks\*), they do not provide a common framework for solving different classes of problems in a systematic manner, nor do they in general guarantee optimality. Furthermore, one particular aspect where these approaches have an important limitation is in accounting explicitly for the interactions that take place when synthesizing total processing systems that consist of several major components, such as the utility system, heat recovery network and chemical plant (Papoulias [10]).

As will be shown in this series of three papers, some of the above cited limitations can be circumvented with an approach based on mixed-integer linear programming, a technique that allows simultaneous structural and parameter optimization in process synthesis. Also, with mixed-integer programming one can develop a common mathematical framework for different synthesis subproblems and having this representation, one can interconnect the subproblems in a natural way to account for the interactions. It is important to note that the suggested approach does not preclude in any way the use of heuristics or thermodynamic targets. Since in the mixed-integer approach a superstructure must be postulated that has embedded many alternative flowsheets, heuristics and thermodynamic targets can be incorporated to reduce the space of search, which in a number of instances will reduce significantly the computational requirements. However, it is clear that the mixed-integer programming approach can only guarantee optimality with respect to the alternatives that are included in the superstructure.

This paper addresses explicitly the problem of synthesizing optimal utility systems that have to satisfy fixed demands of electricity, power for drivers and steam at various pressure levels. A mixed-integer linear programming model is developed which as will be shown in the third part of these papers [12], can be incorporated readily in the synthesis of total processing systems that consist of the chemical plant, heat recovery network and utility system.

#### Conclusions and Significance

A mixed-integer linear programming model has been developed for the systematic synthesis of utility systems. It was shown that considerable advantage can be taken from the flowsheet topology and consistency of operating conditions for introducing only a modest number of binary variables in the formulation. Therefore, as demonstrated with the numerical example, large problems can be solved with reasonable computational effort. Also, the numerical example has shown that alternatives that are potentially attractive for utility systems need not be discarded with the proposed approach.

## Introduction

The objective of this series of three papers is to present a structural optimization approach for the synthesis of total processing systems. A total processing system can be regarded as an integrated system, consisting of three interactive components:

- a) Chemical Plant
- b) Heat Recovery Network
- c) Utility System

The chemical plant is the component that performs the processing steps to transform raw materials into products so as to meet given design specifications. In most cases there are many potential flowsheets for the chemical plant that include a variety of processing units such as reactors, compressors, distillation columns and absorbers, all of which can be interconnected in many different ways. The heat recovery network has the task of exchanging heat among hot and cold process streams of the chemical plant in order to reduce the heating and cooling utilities. The optimal synthesis of this component is often crucial in determining the energy efficiency of the total system. Finally, the utility system provides the required utilities for the chemical plant (electricity and power to drive process units), and heating utilities for the heat recovery network (steam at different pressure levels). Typical units found in a utility plant are fired or waste heat boilers, different types of turbines, electric motors, electric generators, and other auxiliary power plant units. All these units can usually be combined in many feasible configurations that are capable of providing the required utility demands.

In this paper a general mathematical framework based on mixed-integer linear programming will be presented for synthesizing the above cited components. The distinct feature of the proposed approach is that it allows simultaneous

structural and parameter optimization for the optimal synthesis. The application of this approach will be illustrated in this paper with the synthesis problem of utility systems. Part II [11] of this series of papers will deal with heat recovery networks which have a special structure that can be exploited for an efficient solution. Finally, in Part III [12] it will be shown that a mixed-integer formulation of the chemical plant provides a natural way of interconnecting it with the heat recovery network and the utility system, since the formulation can account explicitly for the interactions that take place in the synthesis of the total processing system.

#### Mixed-Integer Programming Approach

In the synthesis of a processing system it is necessary to select the configuration and operating conditions of a flowsheet that optimizes a given objective function while satisfying the required design specifications. In the initial stages of design the objective function is commonly economic in nature and involves either cost minimization or profit maximization. In order to perform both the structural and parameter optimization, the synthesis problem can be formulated as a mixed-integer optimization problem as discussed in Grossmann and Santibanez [3].

The first step in formulating such a problem involves the derivation of a general configuration or superstructure that has embedded all the alternative flowsheets that are to be considered, and from which the optimal solution will be selected. This superstructure contains a finite number of processing units with their corresponding interconnections. The superstructure is commonly derived by making use of engineering judgement, heuristics and/or thermodynamic considerations. The following variables can be associated with the superstructure:

- a) The  $n_y$  - vector  $y$  of 0-1 binary variables associated with the non-existence or existence of units that will define the configuration of the process.



b) The  $n_x$  - vector  $x$  of continuous variables which correspond to stream flowrates, operating conditions and sizes of units.

The physical performance of the superstructure can be represented by the system of linear and nonlinear equations,

$$\begin{aligned} A x &= a \\ f(x) &\gg 0 \end{aligned} \tag{1}$$

where  $A$  is a matrix of constant coefficients with the vector  $a$  as its right-hand side, and  $f$  is the vector of nonlinear equations. In general the system of equations in (1) will be underdetermined leaving a positive number of degrees of freedom. The design specifications, physical constraints, and relations for the layout of possible processing systems which may be expressed in terms of the 0-1 binary variables  $y$ , have the general form:

$$\begin{aligned} b^L &\leq B_1 x + B_2 y \leq b^U \\ h^L &\leq h(x,y) \leq h^U \end{aligned} \tag{2}$$

where  $B_1$ ,  $B_2$  are matrices of constant coefficients,  $b^L$  and  $b^U$  are lower and upper bounds, and  $h$  is the  $m$ -vector of nonlinear constraints with lower and upper bound  $h^L$ ,  $h^U$ .

If the cost function  $C$  to be minimized is given by

$$\min C \ll C(x,y) \tag{3}$$

the synthesis problem consists in determining the optimal values of the variable vectors  $x$  and  $y$  in the following mixed-integer nonlinear program (MINLP):

$$\begin{aligned} \min C &= C(x,y) \\ \text{s.t.} & \\ Ax &= a \\ f(x) &= 0 \\ b &\leq B_1 x + B_2 y \leq b^U \\ h^L &\leq h(x,y) \leq h^U \\ x_j &\geq 0 \gg y_j \in \{0,1\} \quad j = 1,2,\dots,n_y \end{aligned} \tag{4}$$

Due to the difficulty involved in solving this large-scale MINLP Grossmann and Santibanez [3] have suggested to reformulate (4) as a mixed-integer linear program (MILP). This is a class of problems for which efficient algorithms are available for large-scale problems (see Geoffrion and Martsen [2]; Tomlin [17]), and they have the important property of determining global optimum solutions. The MILP formulation for process synthesis can be derived with the general procedure described below.

In order to convert the functions  $f$ ,  $h$ , in linear forms, advantage can be taken from the fact that if operating conditions such as pressures, temperatures, split fractions or other state parameters have fixed values, linear equations can be derived for the performance of each unit (material and energy balances, design specifications, physical constraints, etc.). 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:

- a) The  $n_y$ -vector  $y$  of binary variables which indicate the existence or non-existence of units and streams, and which define the configuration of the process.
- b) 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.
- c) 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:

$$\begin{aligned}
 E_1 y^d + E_0 x^c & \geq e \\
 d & \leq D_1 y + D_2 y + D_3 x^d
 \end{aligned}
 \tag{5}$$

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. 1, 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:

$$\begin{aligned}
 C_j(y, x_j) &= a_j y_j + g_j x_j \\
 x_j^L y_j &\leq x_j \leq x_j^U y_j
 \end{aligned}
 \tag{6}$$

This fixed charge cost function reflects economies of scale since a fixed charge  $a_j$  for the investment of plant unit  $j$  is only incurred when the associated binary variable is set to 1, or equivalently when the unit capacity is greater than zero in which case the variable cost term  $g_j x_j$  is activated. Furthermore, lower and upper bounds on the capacity of units ( $x_j^L$  and  $x_j^U$ ) can be specified in order to reduce the error between the fixed charge cost function and the actual concave cost function as shown in Fig. 1. Also, if a more accurate approximation is desired, more than one binary variable can be used to approximate the concave cost function as a piecewise linear function [15].

Therefore, the general 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):

$$\begin{aligned}
 \min \quad C &= (\alpha_1)^T y + (\alpha_2)^T y^d + (\beta)^T x^c \\
 \text{s.t.} \quad E_x y + E_2 x^c &\leq e \\
 d^L &\leq D_x y + D_2 y^d + D_3 x^c \leq d^U \\
 y_j &= 0, 1 \quad j = 1, 2, \dots, n_y \\
 y_j^d &= 0, 1 \quad j = 1, 2, \dots, a_y^* \\
 x^c &\geq 0
 \end{aligned} \tag{7}$$

where  $C$  is the cost function,  $y, y^d$  are binary vectors and  $x^c$  is the vector of continuous variables;  $\alpha_1, \alpha_2, \beta, 0$ , 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.

### Synthesis of Utility Systems

In order to illustrate the application of the MILP formulation for process synthesis, the problem of utility systems will be considered. This synthesis problem can be stated as follows. A chemical complex requires 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 then to determine the configuration and operating conditions of a utility plant that satisfies the given set of demands at minimum cost. Since in general many alternative types and arrangements of energy supply and conversion devices have to be considered, it is a nontrivial task to synthesize the minimum cost configuration. Few methods have been suggested previously in the literature for synthesizing optimal utility systems, and they are briefly described below.

An iterative linear programming (LP) model was developed by Nishio and Johnson [8] in order to synthesize optimal steam and power plants. One of the shortcomings in their approach is that some major decisions on the plant configuration are based on heuristic rules that exclude many alternatives that could possibly contain the optimal solution. Another important limitation is that the investment costs are considered to be strictly linear with capacities, and hence the economies of scale are not reflected in this model which can produce designs that contain too many units. In a more recent work Nishio et al. [9] proposed a thermodynamic approach. This method attempts to create a utility plant that minimizes available energy losses for each plant unit, and then allocates process drivers (turbines, electric motors) using linear programming. The thermodynamic analysis of available energy is the basis in deriving a set of heuristic rules that will be used to determine the plant structure and design conditions. Although minimization of available energy losses leads to maximum plant efficiency, it clearly does not account for the associated investment costs of the utility plant units. Furthermore, in this method it is not always clear what the precedence of one heuristic rule is over another.

Grossmann and Santibanez [3] have formulated the synthesis problem of steam generation systems as a mixed-integer linear program. Although their model accounts for different operating conditions (pressures and temperatures), it is rather simplified since it does not consider turbine and motor driver assignments for satisfying electricity and power demands, nor heat integration improvements of the plant cycle. The driver assignment problem is very important in the synthesis of optimal steam and power systems since in general it is not known a priori which power demands will be satisfied by high or medium pressure steam turbines, gas turbines or electric motors. Recently,

Petroulas and Reklaitis [13] proposed a synthesis procedure for utility systems based on a decomposition of two coupled subproblems. The first subproblem determines the number of steam headers as well as the pressure in each header, and is modeled as a dynamic program that minimizes the available energy losses. The driver selection is the second subproblem, and is formulated as a linear program having as objective to minimize the energy inputs to the utility plant (steam and electricity). Coupling of the two subproblems occurs at the driver efficiencies and heat load of the boiler. The limitation of this procedure is that it does not account for investment costs of the plant units and does not consider the possibility of using gas turbine drivers. Also the LP formulation for the driver selection problem may not be adequate in many cases, since it might give designs having steam turbines with an excessive number of extractions and inputs, or select two different drivers (steam turbine and electric motor) for satisfying the same power demand. As shown below, the problem of synthesizing utility systems can be formulated as a MILP that can overcome some of the limitations or difficulties encountered in the above cited methods.

#### Derivation of the Superstructure

The first step in the formulation of the synthesis problem of utility systems is to consider systematically many alternative configurations by including them in a superstructure. In this general flowsheet all common units employed in a utility plant are included, namely, boilers generating steam, different types of turbines generating power and electricity, electric motors converting electricity to power, steam headers at different pressure levels, condensers and other auxiliary equipment discussed below. A superstructure for a utility system, containing a very large number of feasible alternative designs is presented in a simplified form in Fig. 2.

Observe that there are three steam headers at high, medium and **low** pressure levels respectively. In each pressure level different steam pressures and temperatures (states) can be considered, but 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 reducers 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 operate in either a high or medium pressure level depending on the inlet pressure of the steam. 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, [14]). 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. It should be noted that the amount of electricity generated is not always the demand specified by the problem, since it may be necessary to produce additional electricity to drive electric motors for satisfying some of the power demands.

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. here 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. Finally, provisions should be made for satisfying the utility plant power requirements (internal demands), for the feedwater pump, boiler draft fans and cooling water pumps.

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 stream 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. The criterion used for optimization in this case is the minimization of the total annual cost of the system.

#### MILP model

Having developed the superstructure for the utility system, the second step is to formulate the synthesis problem as a mixed-integer linear program. In order to develop this MILP model continuous and binary variables are associated with the general flowsheet presented in Fig. 2. The continuous variables represent the capacities of all the units and stream flowrates (air, hot gases, fuel, steam and water). The binary variables (0-1 variables) assigned to plant units represent the existence or nonexistence of the corresponding units at a given operating state. The operating pressures and temperatures to be analyzed are treated as a set of discrete values with each of them associated to binary variables that indicate the existence or non-existence of the discrete value.



In order to derive the MILP model, consider that in the superstructure the set of units  $N = \{n\}$ , is postulated for providing the given set of utility demands. These processing units are boilers, steam headers at different pressure levels, different types of turbines, pressure reducers and auxiliary power plant units. The first task is to define the interconnections of each plant unit  $n$  with the following index sets:

$$\begin{aligned} I_n &= \{m \mid \text{unit } n \text{ has input flowrate from unit } m\} \\ O_n &= \{m \mid \text{unit } n \text{ has output flowrate to unit } m\} \end{aligned} \quad (8)$$

Therefore, the superstructure for the utility plant can be represented as a mathematical graph (network), where the nodes of the graph are the plant units and the edges are the stream flowrates.

In order to investigate a number of different operating conditions, a subset of units  $N_i \subset N$  is chosen where discrete pressures and temperatures are specified. The units  $N_i$  in this model will correspond to the three steam headers, the vacuum condenser and gas turbines. As a result of the selected discretization of conditions on the units  $N_i$ , discrete operating conditions will also occur in the rest of the units of the superstructure. Therefore, the index set  $K_n$  that defines the discrete conditions of the output streams for each unit is defined as

$$K_n = \{k \mid \text{unit } n \text{ operates at condition } (P_{nk}, T_{nk})\} \quad n \in N \quad (9)$$

The existence or non-existence of unit  $n$  operating at condition  $k$  can then be represented by the binary variables  $y_{nk}$  which are defined as follows:

$$y_{nk} = \begin{cases} 1 & \text{unit } n \text{ is selected in the final structure and} \\ & \text{operates at condition } k \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

As will be shown below, many of these binary variables can actually be eliminated in the implementation of the MILP model by taking advantage of the

topology and consistency of operating conditions in feasible configurations.

As for the continuous variables, the flowrates of the streams in the superstructure will be represented by the non-negative variables  $F_{nk}^m$ , that denote the output flowrate from unit n at condition k, and that is directed to unit m. Each one of these variables will have associated to it the specific enthalpy  $h_{nk}^m$  as a fixed parameter. The heat and work generated by unit n are denoted as  $Q_n$  and  $W_n$  - Therefore, the material and energy balances for all plant units will be given by:

$$\begin{aligned}
 & \sum_{L} y_{meI_n} \sum_{L} y_{keK_m} F_{ink}^n - \sum_{U} y_{meO_n} \sum_{L} y_{keK_n} F_{t_{nk}}^m - 0 \\
 & \sum_{LJ} y_{meI_n} \sum_{U} y_{keK_n} F_{ink}^n \cdot h_{mk}^n - \sum_{LJ} y_{meI_n} \sum_{U} y_{keK_n} F_{ink}^n \cdot h_{nk}^m - 0 - w_n = 0 \quad n \in N \quad (11)
 \end{aligned}$$

In order to activate the flowrates in the superstructure that are consistent with the selection of units and their corresponding operating conditions, logical constraints must be imposed. Firstly, since for each plant unit at most one operating condition k can be selected the following (in)equalities apply,

$$\sum_{keK_n} y_{nk} \leq 1 \quad n \in N \quad (12)$$

In the case that unit n must exist in the final solution the equality is used, whereas in the case when unit n may not exist the inequality is used. To ensure that the output flowrates of each unit are at the same operating condition k if unit n exists, the following inequalities must be included

$$\sum_{meO_n} U \quad (13)$$

where U is an arbitrary upper bound on the stream flowrates.

There are in addition two other types of logical constraints that must hold in the superstructure. The first one arises when a unit  $m$  will exist at the condition  $k$ , if and only if unit  $n$  exists at the same condition. In this case one can set for the corresponding binary variables of units  $m$  and  $n$  the equality

$$y_{mk} = y_{nk} \quad k \in K_n \quad (14)$$

An example of this case would be the relation of the boiler and steam header at high pressure when both must exist simultaneously, and therefore at the same condition.

The second type of constraint arises when the existence of a unit  $m$  at condition  $k$  implies the existence of unit  $n$  at the same condition, but the reverse is not true. In this case only one binary variable  $y_{mo}$ , is required to denote the existence of unit  $m$  and therefore one can set

$$y_{mo} = y_{mk} \quad k \in K_m \quad (15)$$

where  $y_{mo}$  is related to the existence of unit  $n$  by the constraint

$$y_{mo} - \sum_{k \in K_n} y_{nk} \leq 0 \quad (16)$$

Since unit  $n$  will then define the operating conditions at unit  $m$ , constraint (13) must be replaced by the following inequalities to activate the flowrates in unit  $m$

$$\sum_{l \in O_m} F_{mk}^l - U y_{nk} \leq 0 \quad k \in K_n \quad (17)$$

$$\sum_{k \in K_n} \sum_{l \in O_m} F_{mk}^l - U y_{mo} \leq 0$$

An example of this second case would be the relation of a turbine with a steam header, where the existence of the former implies the existence of the latter, but not vice versa.

It is very important to note that it is the equalities in (14) and (15) that allow the elimination of a large number of binary variables in the implementation of the MILP model. The equation in (14) allows the use of the same binary variables for several units, whereas the equation in (15) requires that some units be assigned only one binary variable even if they can operate at several conditions. Using these equalities the only binaries required in the superstructure of the utility plant are for each state of the steam headers and one for each potential steam and gas turbine and electric motor\*

In order to meet the utility demands the continuous variables in the model must meet the following constraints:

a) Power demands

$$W_p = \sum_{n \in N_p} W_n \quad p = 1, 2, \dots, P \quad (18)$$

where  $N_p = \{n \mid \text{unit } n \text{ supplies power demand } p\}$

b) Steam demands (in the form of heat duties)

$$\hat{Q}_s = \sum_{n \in N_s} Q_n \quad s = 1, 2, \dots, S \quad (19)$$

where  $N_s = \{n \mid \text{unit } n \text{ steam demand } s\}$

c) Water demands

$$F_r = \sum_{n \in N_r} \sum_{k \in K_n} F_{nk} \quad r = 1, 2, \dots, R \quad (20)$$

where  $N_r = \{n \mid \text{unit } n \text{ supplies water demand } r\}$

Logical constraints in terms of binary variables can of course also be added to ensure that a given demand is satisfied by only one unit. An example would be when only one turbine should satisfy the power demand for a driver.

As for the capacities of the unit  $n$ , they will be given depending on the type by

$$G_n = \begin{cases} \sum_{meO} V_n & \sum_{keK} V_n & F_{nk}^m & \text{flowrate capacity of unit } n \\ W_n & & & \text{work load of turbine or motor drive } n \end{cases} \quad (21)$$

These capacities will in general be bounded by minimum and maximum capacities  $G_n^L, G_n^U$ , in the constraint

$$G_n^L \langle I_{keK_n} * \bullet * \rangle * G_n * G_n^U \langle I_{keK_n} * nk \rangle \quad (22)$$

Finally, the objective function in the synthesis model is given by the fixed and variable cost of all plant units, while the operating cost is given by the fuel, water or any other purchased utility cost. Therefore, the form of the objective function is •

$$\min C = \sum_{neN} Y_U Y_L (a_{nk} Y_{nk}^i + \sum_{n} B_n G_n) + \sum_{neN} L^Y \sum_{keK} V_{nk}^i F_{nk}^i + \sum_{neN} \sum_{n} W_n \quad (23)$$

where  $N_{TT}$  and  $N_{ei}$  define the units that purchase utilities, and

$a_{nk}, B_n, Y_{nk}^i, W_n$  are cost coefficients,

The problem of synthesizing an optimal utility system given by the objective function (23) and the set of constraints (10)-(22), corresponds to a KLLP for which both structural and parameter optimization can be performed in the superstructure. To obtain the values of the coefficients in the MILP model the following information is necessary:

- a) Data on the utility demands
- b) Enthalpy and entropy data for steam and gas stream
- c) Efficiencies of turbines
- d) Cost correlations for all units and utilities

This MILP model can then be solved with standard mixed-integer programming codes so as to provide the optimal configuration from a superstructure that has embedded many feasible utility systems.

### Numerical Example

In order to demonstrate the application of the MILP model for synthesizing utility systems, a test problem taken from Nishio et al. [9] is considered. 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 1. 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 deaerated and cooling water. Also there is import of medium and low pressure steam and condensate return. The operating conditions and other parameters of the utility plant units are given in Table 2. Note that three operating conditions are considered for each, the high pressure (HP) steam header, and the medium pressure (MP) header. Cost coefficients were derived in the fixed charge form using the cost data given in Guthrie [4] and Woods et al. [19], which were updated to 1981 prices using the Chemical Engineering Index. Stream enthalpies and entropies were obtained from thermodynamic tables ([1], D14), and the turbine efficiencies are the ones given in Nishio et al. [9].

There were two cases studied using the data of 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. [9], 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 same fuel (kerosene) was used for the fired boiler and gas turbine. 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 [15].

The optimal configuration obtained in the first case has an annual cost of 26.82 M\$/year and is shown in Fig. 3. The internal power demands of this optimal design are given in Table 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. Observe that the operating condition with the higher pressure ( $P = 96.53$  bar,  $T = 713^{\circ}\text{K}$ ) is selected for the HP steam header, while the MP steam header operates at the intermediate pressure ( $P = 17.24$  bar,  $T = 600^{\circ}\text{K}$ ). In fact this configuration is similar to the solution given by Nishio et al. [9] with the exception that in the optimal design of Fig. 3 steam reheating ( $68.27 \times 10^6$  kJ/hr) is performed in the boiler. More detailed comparisons among these two solutions (fuel consumption, plant efficiency) are perhaps not appropriate since the values assumed for stack temperature of the boilers are probably different.

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. 4. 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 condition with intermediate pressure ( $P = 69 \text{ bar}$ ,  $T = 661^{\circ}\text{K}$ ) is selected for the HP steam header. Finally, it is important to note that this optimal binary cycle plant has 37.47% less fuel consumption with respect to the above design that uses no gas turbine generator. Clearly, the reduced fuel consumption of the binary cycle represents a significant improvement in the efficiency of the utility system.

#### Discussion

As shown with the numerical example, the MILP approach is a powerful tool for designing utility systems. The fact that potentially promising alternatives can be embedded in the superstructure and that they need not be discarded has produced in the above example savings of 37.47% 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. 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 in the third part of this series of papers [11].



Another point worth mentioning from the examples that were solved is that the proposed MILP model for utility systems constitutes an efficient synthesis method since modest computational effort was required for solving both cases of the example problem (less than 2 minutes CPU time on a DEC-20). For larger problems, it would be possible to decrease the computational effort for solving this MILP problem by adding heuristic constraints to the proposed formulation that will reduce significantly the feasible region, and hence the enumeration effort. For the synthesis of utility systems, an appropriate heuristic constraint would be to specify that the maximum fuel cost, which is the dominant term in the annual cost, is within a small percentage (e.g. 5%) of the value obtained at the relaxed LP solution. The effect of this constraint in the MILP model is to eliminate from consideration utility plant configurations with fuel consumption that most likely will not lead to the optimal solution. However, care should be taken in the use of this constraint as too small a percentage may not produce any feasible solutions.

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## References

- [1] Babcock and Wilcox Co., Steam. Its Generation and Use, Babcock and Wilcox Co., New York (1978).
- [2] Geoffrion, A.M. and R.E. Marsten, "Integer Programming Algorithms: A Framework and State-of-the-Art Survey"<sup>11</sup>, Manage. Sci., 18, 17 (1972).
- [3] Grossmann, I.E. and J. Santibanez, "Applications of Mixed-Integer Linear Programming in Process Synthesis"<sup>11</sup>, Computers and Chem. Eng., 4, 205 (1980).
- [4] Guthrie, K.M., Process Plant Estimation, Evaluation and Control, Craftsman Book Co., Solana Beach (1974).
- [5] Hendry, J.E., D.F. Rudd and J.D. Seader, "Synthesis in the Design of Chemical Processes", AIChE J., 19, 1 (1973).
- [6] Hlavacek, V., "Journal Review: Synthesis in the Design of Chemical Processes", Computers and Chem. Eng., 2, 67 (1977).
- [7] Nishida, N., G. Stephanopoulos and A.W. Westerberg, "Journal Review: Process Synthesis", AIChE J., 27, 321 (1981).
- [8] Nishio, M. and A.I. Johnson, "Strategy for Energy System Expansion", Chem. Eng. Prog., 73, 75 (1979).
- [9] Nishio, M., J. Itoh, K. Shiroko and T. Umeda, "Thermodynamic Approach to Steam and Power System Design", Ind. Eng. Chem. Process Des. Dev., 19, 306 (1980).
- [10] Papoulias, S.A., "Studies in the Optimal Synthesis of Chemical Processing and Energy Systems"<sup>11</sup>, Ph.D. Thesis, Carnegie-Mellon University, Pittsburgh (1982).
- [11] Papoulias, S.A. and I.E. Grossmann, "A Structural Optimization Approach in Process Synthesis. Part II: Heat Recovery Networks", submitted for publication (1982).
- [12] Papoulias, S.A. and I.E. Grossmann, "A Structural Optimization Approach in Process Synthesis. Part III: Total Processing Systems", submitted for publication (1982).
- [13] Petroulas, T. and G.V. Reklaitis, "Computer-Aided Synthesis and Design of Plant Utility Systems", paper 51c presented at the National AIChE Meeting, Houston (1981).
- [14] Sawyer, J.W. (ed.), Gas Turbine Engineering Handbook, Gas Turbine Publications, Inc., Stamford, Conn. (1966).
- [15] Schrage, L.E., User's Manual for LINDO, The Scientific Press, Palo Alto (1981).
- [16] Stephanopoulos, G., "Synthesis of Process Flowsheets: An Adventure in Heuristic Design or a Utopia of Mathematical Programming?", in R.S.H. Mah and W.D. Seider (eds.), Foundations of Computer-Aided Chemical Process Design, Vol. 2, p. 439, Engineering Foundation, New York (1981).

- [17] Tomlin, J.A., "Large Scale Mathematical Programming Systems", paper presented at the AIChE Annual Meeting, Los Angeles (1982).
- [18] Westerberg, A.W., "A Review of Process Synthesis", ACS Symposium Series, 124, (1980).
- [19] Woods, D.R., S.J. Anderson and S.L. Norman, "Evaluation of Capital Cost Data: Offsite Utilities", Canadian J. Chem. Eng., 53, 533 (1979).

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 POWER		
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 POWER		
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/h r

Table 2: Stream/Equipment Conditions for Example Problem

STREAM/EQUIPMENT	CONDITIONS
<b>H.P. STEAM HEADER</b>	
Operating Condition no. 1.....	P = 96.53 bar, T <sup>s</sup> 713 K
Operating Condition no. 2.....	P = 68.95 bar, T << 661 K
Operating Condition no. 3.....	P * 55.16 bar, T = 782 K
<b>M.P. STEAM HEADER</b>	
Operating Condition no. 1.....	P = 20.68 bar, T * 758 K
Operating Condition no. 2.....	P = 17.24 bar, T << 600 K
Operating Condition no. 3.....	P = 13.79 bar, T >> 690 K
<b>L.P. STEAM HEADER</b>	
Operating Condition no. 1.....	P = 3.45 bar, T = 411 K
<b>DEAERATOR</b> .....	pressure = 1.013 bar temperature = 373 K
<b>FEEDWATER HEATER</b> .....	heat donor (M.P. steam) heat receiver (BIW)
<b>BOILER</b> .....	blow-down rate = 5% efficiency ≈ 90% fuel LHV = 43950 kJ/kg fuel cost = 0.1395 \$/kg
<b>VACUUM CONDENSER</b> .....	exhaust steam pressure ≈ 120 mmHg condensate temperature = 328 K cooling water in = 303 K cooling water out = 323 K
<b>COOLING WATER PUMP</b> .....	inlet pressure = 1.013 bar outlet pressure = 7.94 bar inlet temperature = 303 K pump efficiency = 65%
<b>GAS TURBINE GENERATOR</b> .....	compression ratio << 10*0 expansion ratio = 9.8 compressor efficiency = 85% turbine efficiency = 87% combustor efficiency = 98% fuel LHV = 43950 kJ/kg fuel cost = 0.1395 \$/kg max. regenerator eff. <sup>s</sup> 80% exhaust gas temperature >> 900 K

Table 3: Economic Data for Example Problem

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Annual Operation	=	8400 hours
Capital Recovery Factor	=	0.154252
Gas Turbine Fuel (Kerosene)	=	\$ 143/ton
Fired Boiler Fuel (Kerosene)	=	\$ 143/ton
Water	=	\$ 0.05/1000 gallons

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Table 4. Optimal Internal Power Demands for Example Problem

INTERNAL POWER	CALCULATED DEMAND
<b>CASE I: UTILITY SYSTEM WITHOUT GAS TURBINE GENERATOR</b>	
no. 12 (BFW pump).....	.857 kW
no. 13 (boiler draft fan).....	.879 kW
no. 14 (cooling water pump).....	.2539 kW
<b>CASE II: UTILITY SYSTEM WITH GAS TURBINE GENERATOR</b>	
no. 12 (BFW pump).....	.326 kW
no. 13 (boiler draft fan).....	.239 kW
no. 14 (cooling water pump).....	.1827 kW

Figure 1. Approximation of concave cost function with fixed-charge cost function.

Figure 2. Superstructure of utility system.

Figure 3. Optimal utility system with no gas turbine generator.

Figure 4. Optimal utility system with gas turbine generator.



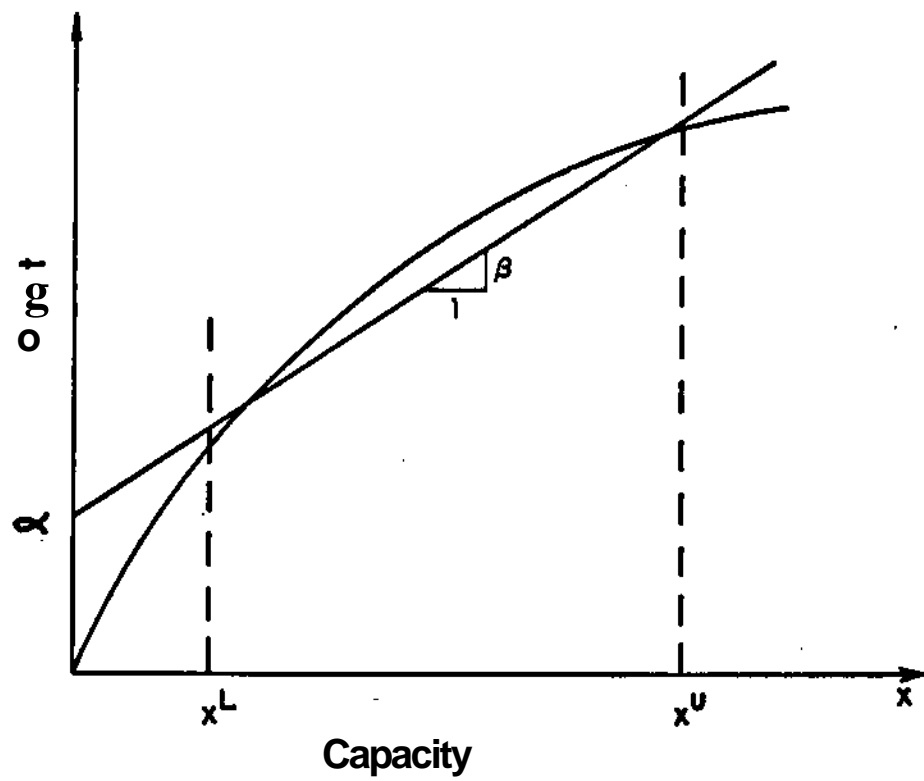


Fig. 1

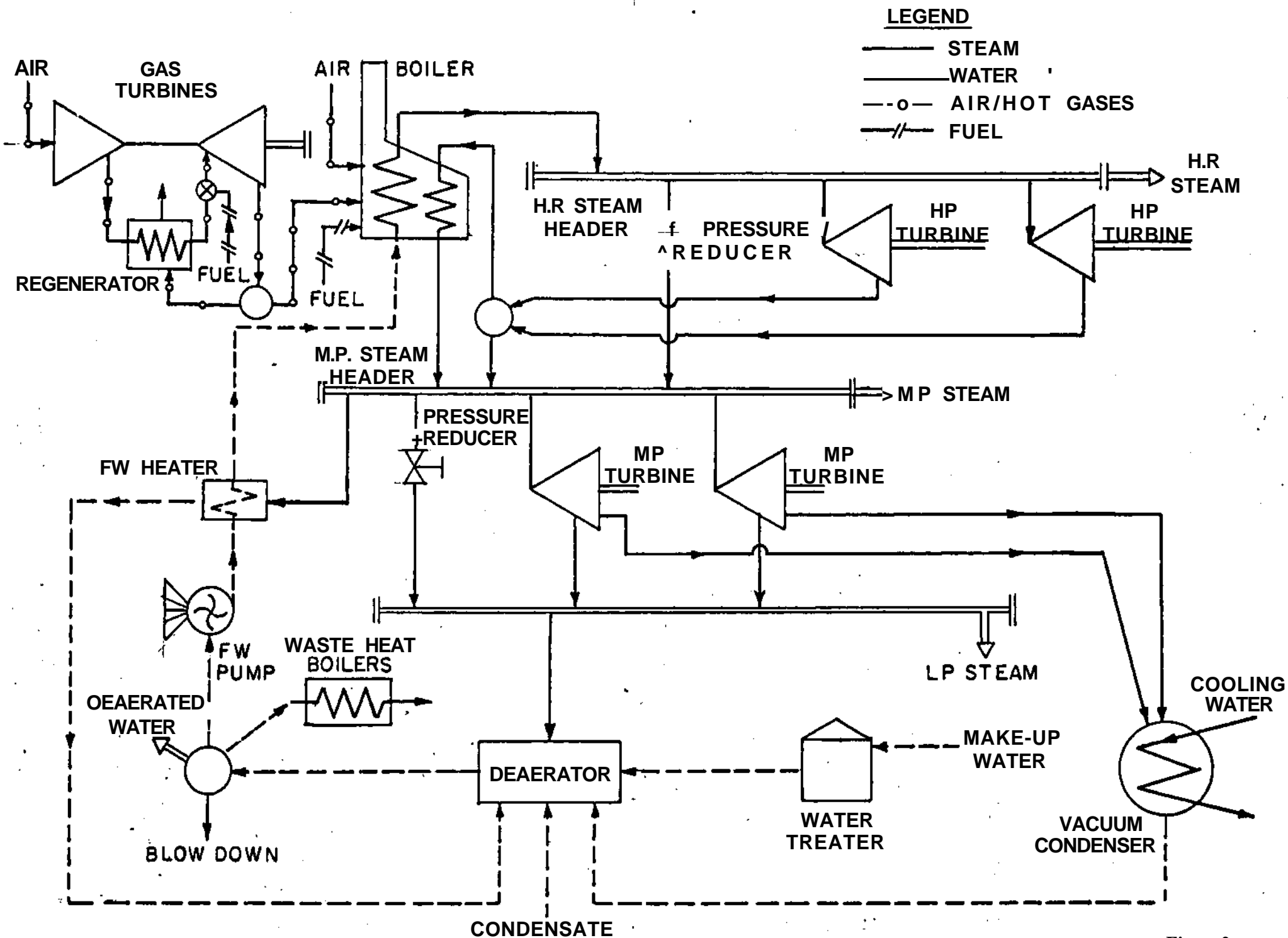


Fig. 2



**ELECTRIC MOTORS (KW)**

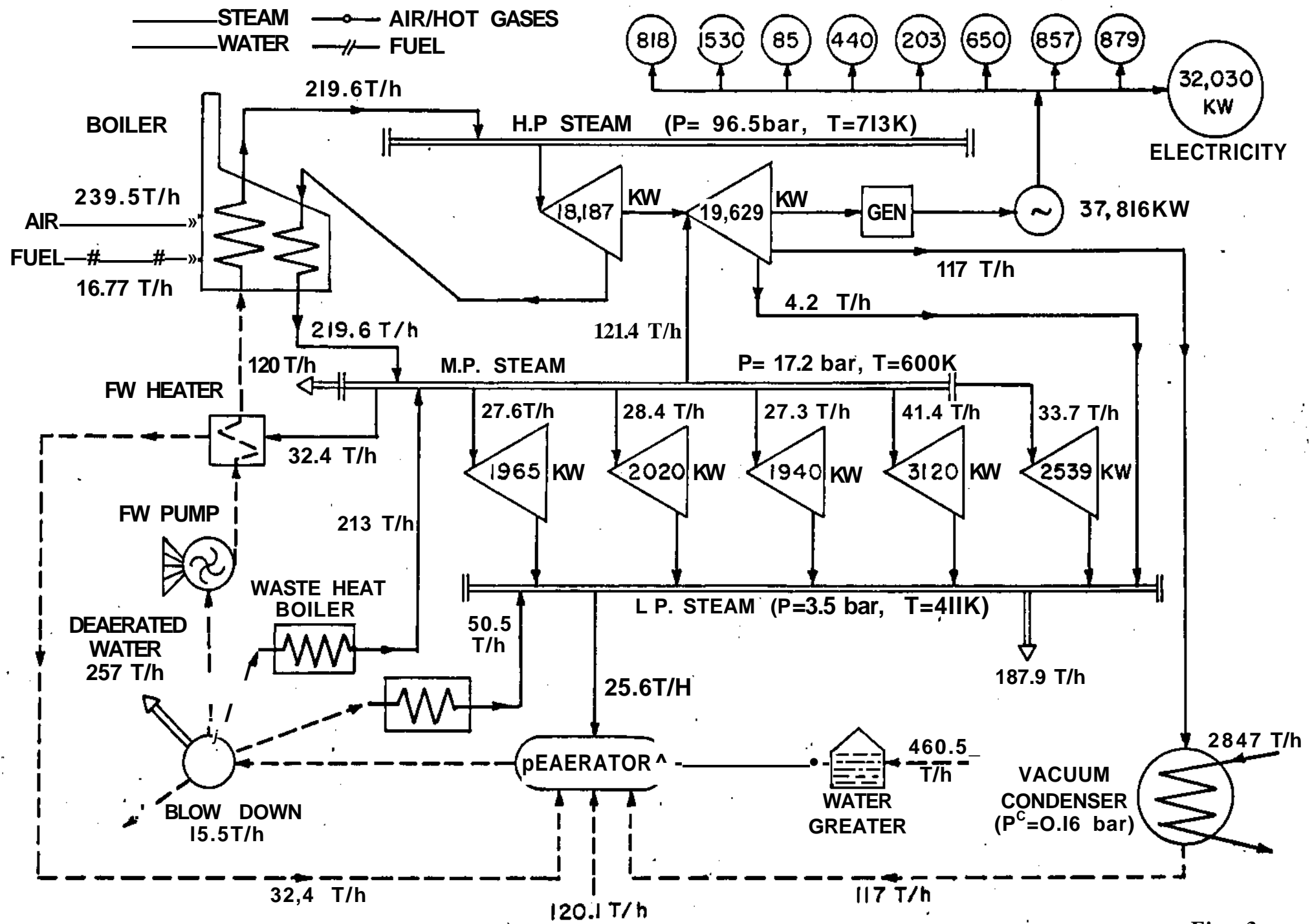


Fig. 3

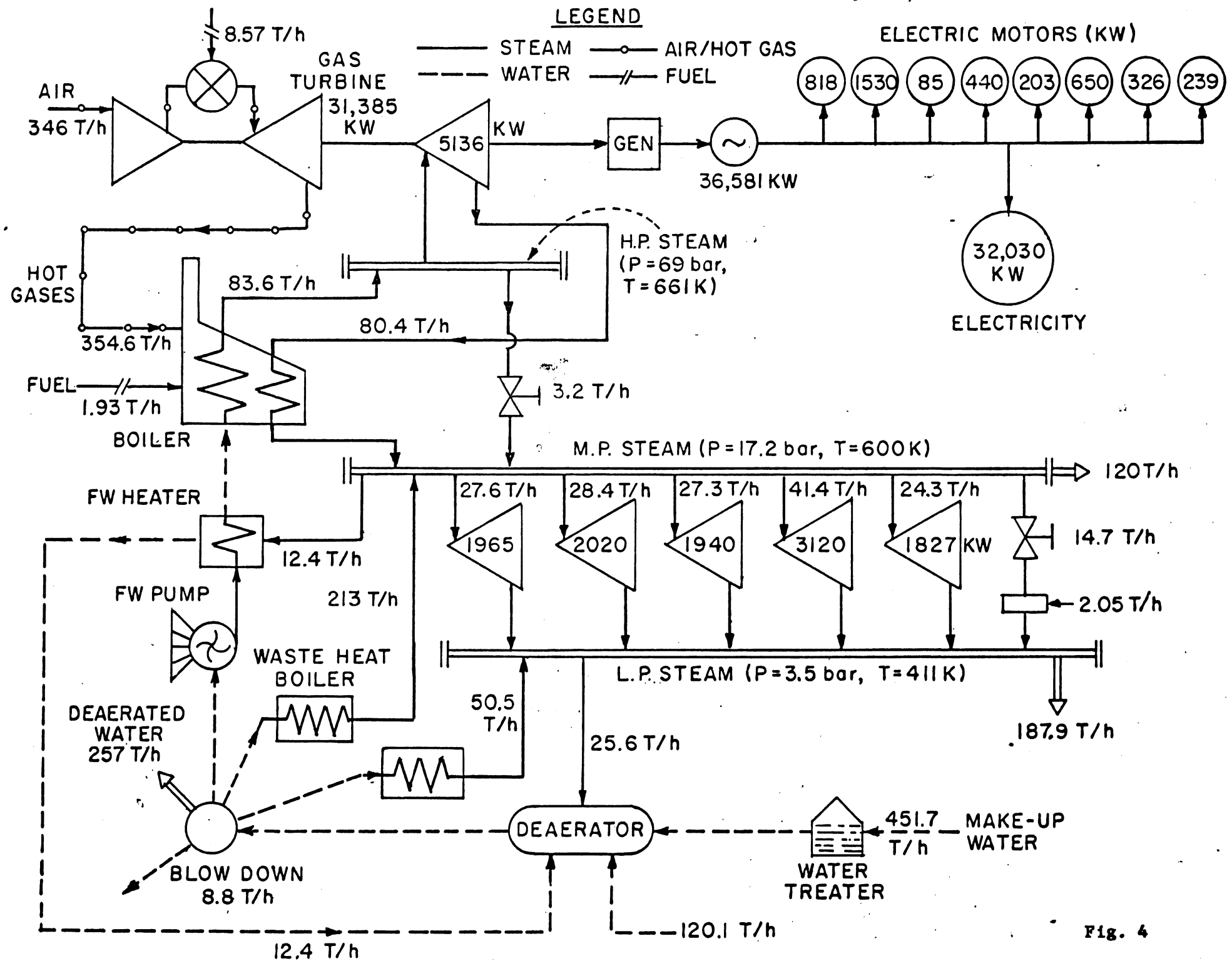


Fig. 4