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X STRUCTURAL OPTIMIZATION APPROACH IS PROCESS SYNTHESIS
PART III: TOTAL PROCESSING SYSTEMS

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A STRUCTURAL OPTIMIZATION APPROACH IN PROCESS SYNTHESIS. PART III: TOTAL PROCESSING SYSTEMS

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Abstract

A strategy based on mixed-integer programming is proposed for the optimal synthesis of total processing systems that consist of a chemical plant, with its heat recovery network and utility system. A mixed-integer programming model for the chemical plant is presented which is shown to be compatible with the models developed in previous papers for the utility system and heat recovery network. The strategy accounts explicitly for the interactions among the three components, and its application is illustrated with a large example problem.

Scope

Two major classes of methods have been proposed for the systematic synthesis of chemical plants [7]. One class encompasses methods that synthesize plants without requiring an initial structure, while the other class of methods extract the optimal configuration from a superstructure that has embedded a number of design alternatives. In the first type of methods artificial intelligence techniques have been applied, as for instance in the AIDES program (Siirola et al. [12]) with the general problem solver principle, and in the BALTAZAR program (Mahalec and Motard [4], [5]) with the mechanical proving theorem. On the other hand, in the second type of methods nonlinear optimization techniques have been applied to small problems by a number of researchers (Umeda et al. [14], Ichikawa and Fan [2], Osakada and Fan [8], Stephanopoulos and Westerberg [13], Nishida and Powers [6]). The limitations of the methods based on artificial intelligence is that they rely heavily on the use of heuristic rules, whereas the methods based on nonlinear optimization techniques give rise to large-scale nonconvex problems which in general are very difficult to solve.

It is the purpose of this paper to show that the structural optimization approach can be performed effectively with mixed-integer linear programming (MILP) techniques. A MILP model is presented for the chemical plant which can

be incorporated in a strategy for synthesizing the plant simultaneously with its heat recovery network and utility system. This unique feature which has not been reported previously in the literature, is accomplished with the models presented in the first two papers of this series [9], [lO], The main advantage of the strategy is that the synthesis of the three components can be coordinated in a natural and rigorous way.

Conclusions

A strategy based on mixed-integer programming has been proposed for synthesizing total processing systems. It was shown that with the proposed mathematical framework the optimal synthesis of a chemical plant with its heat recovery network and utility system can be performed simultaneously. This was illustrated with a representative example of a chemical process. The computer time requirements were small showing that the proposed strategy is an efficient screening method for process synthesis.

Introduction

As discussed in the first part of this series of papers [9], a total processing system can be regarded as an integrated system consisting of three main components:

a) Chemical Plant

b) Heat Recovery Network

c) Utility Plant

In the synthesis of such a system a crucial role is played by the interactions among the three basic components as shown in Fig. 1. The interactions among the chemical plant with the heat recovery network are all the cold and hot process streams that require heating and cooling. The interactions among the chemical plant and utility system are the electricity and power demands required in the chemical plant. Finally, the interactions between the heat recovery network and the utility system are the hot utilities (fuel, steam at different pressure levels and hot water) and the cold utilities (cooling water and refrigerants) required for providing the necessary heating and cooling in the heat exchanger network.

Although in recent years there has been considerable progress in understanding and developing synthesis procedures for each subsystem separately, not much attention has been placed in the problem of coordinating the synthesis activity for the three components of the total processing system. As reported recently by Linnhoff and Townsend [3], the usual procedure is to decompose the problem by designing first the chemical plant with any method (mainly heuristics) in order to determine the required values for the interactions with the heat recovery network and the utility system. The next step is then to develop the heat recovery network for the fixed process streams of the chemical plant, so that the minimum heating and cooling utility consumption is calculated. At this point all

interactions between the components are determined, and therefore the design of the total system can be completed with the utility system. The design of the supporting utility system is performed based on the fixed electricity, power, heating and cooling utility demands. Although Linnhoff and Townsend [3] do not offer any method for the synthesis of the total system, they made suggestions about the placement of heat engines and heat pumps of the utility system with respect to the pinch points in the heat recovery network.

It is important to note that the sequential synthesis procedure is seriously handicapped from the fact that the chemical plant is designed without any consideration to heat integration for all process streams requiring heating and cooling. It should be noted that if the synthesis of the chemical plant is performed independently it is possible to account for the cost of electricity and power demands with nominal prices, while the cost of heating and cooling all process streams cannot be determined properly without solving the heat recovery network. This difficulty limits considerably the effectiveness of any synthesis procedure, since the important objective of heat integration is not properly reflected in the evaluation of alternative configurations for the chemical plant. As for the utility system, it is also true that nominal prices may not necessarilly lead to its efficient integration with the chemical plant and heat recovery network. Thus, it is clear that the sequential approach for synthesis may not account properly for the interactions in a total processing system.

In this paper a strategy based on mixed-integer linear programming (MILP) is proposed for the synthesis of total processing systems. A MILP model is presented for the chemical processing plant for which a large number of flowsheet structures can be considered in a systematic manner. It will be shown that this model together with the MILP synthesis model for utility systems and the trans-

shipment model for the heat recovery network, both of which were given in Part I [9] and Part II [10] of this series of papers, can easily be combined in a general mathematical model for the optimal synthesis of total systems. The application of this model will be illustrated with an example problem which is representative of many chemical processes.

Synthesis Strategy for 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 components of the system. This coordination should enable the evaluation of different configurations of the chemical plant, as well as of 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 is proposed for that purpose:

Step 1. A superstructure is developed for the chemical plant which contains for instance different reactors or separation sequences that are to be analyzed* 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 KELP for the chemical plant can be derived using the model that is presented later in the paper.

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 (P3) for minimum utility cost is formulated as discussed in Papoulias and Grossmann [10]. In this model the flowrates of the process streams appear as variables that depend on the actual structure of the chemical plant. Since the transshipment model (P3) does not define explicitly the configuration of the heat recovery network, its

'nvestment 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 is 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 system and its MILP formulation can be derived as discussed in Papoulias and Grossmann [9]. In this case 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 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. It should be noted that although it is desirable to solve this large MILP simultaneously in order to account fully for all the interactions, another option is to first solve the chemical plant and heat recovery network using nominal prices for the utilities, and then having the demands synthesize the utility system. This however, will not necessarily yield an equivalent solution to the simultaneous synthesis method since the selected prices of utilities may not be accurate, and furthermore the integration of the utility system may not be performed efficiently.

Step 5. Having solved the MILP of the total processing system, the solution of the transshipment model (P3) will provide the minimum utility cost for the chosen chemical plant, since heating and cooling utilities provided by the utility 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 (P2) proposed by Papoulias and Grossmann [lO].

The efficiency of this synthesis strategy is clearly dependent on the size of the resulting MILP model for a total processing system. As shown in the two previous papers [9], [10], the MILP model for utility systems and the LP transshipment model for heat recovery networks yield problems of reasonable size. In the next section the MILP model for the chemical processing plant will be presented. As will be shown, this model can also be of reasonable size provided that only selected alternatives are included in the superstructure.

MILP Model for Chemical Plant

As was outlined in the strategy for synthesizing total processing systems the derivation of a superstructure for the chemical plant is required in step 1. This superstructure will typically include reactors, separation columns, compressors and pumps. The heating and cooling tasks in this superstructure will be represented by heating and cooling units which will define the hot and cold streams for the heat recovery network. Although in principle one could consider an extremely large number of alternative flowsheets of the chemical plant in the superstructure, in most cases only a reasonable number would be included. The reason is that in practice the designer would normally consider only selected alternatives that are potentially attractive, since many options would have been discarded a priori by considering practical constraints, past experience, heuristics or thermodynamic arguments. Therefore, the MILP synthesis method proposed in this paper should be regarded as a screening tool for selected alternatives, rather than for all possible chemical reaction paths and all possible separation sequences that could be conceived for the chemical plant.

Having postulated a superstructure for the chemical plant the corresponding MILP model can be derived as follows. The processing units such as reactors, separation columns, compressors and pumps will be denoted by the set $N_P \subseteq \{n\}$, whereas the set of heating and cooling units will be denoted by the set $N_Q = \{n\}$. Therefore, the total set of units is given by N, where $N = N_P \cup N_Q$. The interconnection for these units can then be represented by the following index sets:

$$I_n \subseteq \{m \mid \text{unit } n \text{ has input flowrate from unit } m\}$$
$$O_n \subseteq \{m \mid \text{unit } n \text{ has output flowrate to unit } m\} \quad (1)$$

In general, a subset of units $N^I \subseteq N^P$ can be chosen for investigating discrete operating conditions such as pressures, temperatures, split fractions or conversions. As a result of this discretization, discrete operating conditions will also occur in the remaining units of the superstructure. Therefore, for each unit $n \in N$, one can define the index set K_n of discrete operating conditions of the output streams,

$$K_n = \{k \mid \text{unit } n \text{ operates at condition } (s^1_{nk}, s^2_{nk}, \ldots)\} \quad (2)$$

where $s^1_{nk}, s^2_{nk}, \ldots$, corresponds to the particular values of pressure, temperature, conversion, split fraction, etc. For each heating and cooling unit $n \in N_Q$ it will be assumed that the index set K_n will be identical to the index set of the unit m to which it is directed. That is $K_n = K_m$, $m \in O_n$, $n \in N_Q$.

The existence or non-existence of each unit $n \in N$, can be represented by the binary variable y_{nk} which is defined as follows:

$$y_{nk} = \begin{cases} 1 & \text{unit } n \text{ is selected in the final structure and operates as condition } k \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

Similarly as in the case of utility systems (see Papoulias and Grossmarm [9]) many of these binary variables can actually be eliminated in the implementation of the

MILP model as will be shown below.

The flowrates of each component in the streams of the superstructure will be represented by the non-negative variable F^m_{cnk}. This variable denotes the output flowrate of component c from unit n at condition k, and which is directed to unit m. Each one of these variables will have associated as a fixed parameter the specific enthalpy h^m_{cnk}. The material and energy balances for the set of units N_p is then given by

$$\sum_{m \in I_n} \sum_{k \in K_m} \theta_{cnk} F_{cmk} - \sum_{m \in O_n} \sum_{k \in K_n} F^m_{cnk} = 0 \qquad c \in C, \; n \in N_p \tag{4}$$

$$\sum_{c \in C} \sum_{m \in I_n} \sum_{k \in K_m} F_{cmk} h_{cmk} - \sum_{c \in C} \sum_{k \in O_n} \sum_{k \in K_n} F^m_{cnk} h^m_{cnk} - Q_n - W_n = 0 \quad n \in N_p$$

where θ_{cnk} represents the split fractions of unit n, Q_n and W_n are the heat and work generated at that unit, and C is the set of chemical components. It should be noted that for most cases the use of split fractions for the mass balances will yield reasonably good approximations for nonlinear units, that would be suitable in a preliminary design*

As for the set of heating and cooling units; it is convenient to define the variables $f^{nk}_{cp\ell}$, to denote the flowrate going from a processing unit $p \in N_p$ at condition ℓ, to a heating or cooling unit $n \in N_Q$ at condition k. These variables correspond to the flowrates of hot or cold streams that are to be used in the transshipment model (P3) for minimum utility cost. Note that these variables define explicitly the inlet and outlet temperatures of these streams, and that they are related to the flowrates $F_{cp\ell}$ and F^m_{cnk} by the equalities

$$F^n_{cp\ell} = \sum_{k \in K_n} f^{nk}_{cp\ell} \qquad \ell \in K_p$$

$$F^m_{cnk} = \sum_{\ell \in K_p} f^{nk}_{cp\ell} \qquad k \in K_n \tag{5}$$

In order to activate the flowrates in the superstructure that are consistent with the selection of units and their corresponding operating conditions the following constraints that involve continuous and binary variables must hold (see Papoulias and Grossmann [9]):

a) Selection of unit n at one operating condition k

$$\sum_{k \in K_n} y_{nk} \left[\leq\right] 1 \qquad (6)$$

b) Selection of a non-zero flowrate at only one condition k

$$\sum_{m \in O_n} \sum_{c \in C} F^{m}_{cmk} \text{ " } U y_{nk} * 0 \qquad k \in K_n, \quad n \in N$$

where U is an arbitrary but valid upper bound.

c) Selection of simultaneous units

$$y_{mk} \cdot *_{nk} \qquad k \in K_n \qquad (7)$$

where units m and n must exist simultaneously.

d) Selection of conditional units

$$\text{"}_{mo} = y_{mk} \qquad k \in K_m \qquad (8)$$

$$y_{mo} \cdot I \; y_i < o \qquad (9)$$

$$\sum_{leO_m} \sum_{cec} F'_{cmk} - U y_{nk} \wedge: 0 \qquad k \in K_n \qquad (10)$$

$$\sum_{keK_n} \sum_{m \; cec} i_{cmk} \; y_{a} : 0 \qquad (11)$$

where the existence of unit m implies the existence of unit n, but the converse is not necessarily true.

By making use of the equalities in (7) and (8), the number of actual binary variables can be reduced considerably in the actual implementation of the MILP model. An example where the equality in (7) would be applied is when a compressor is followed by a chemical reactor, both of which would exist simultaneously.

Also, in the case of heating and cooling units N_Q, their existence is determined by the units to which they are connected downstream. Therefore, with the equality in (7) the existence of several units can be represented with the binaries of one single unit. Taking advantage of this fact, none of the heating and cooling units require binary variables to denote their existence. An example of the equality in (8) arises when a second separation column is followed by a first column. Clearly if the second column is selected the first one must also exist, whereas if the first column is selected the second one may not exist if there is the option of selecting a different second column. Therefore, in this case as indicated by eqtns. (8) - (11), some units can be assigned a single binary variable even if they operate at several conditions.

As for the capacities of the units n_e N_p they will be given depending on the type by

$$G_n = \begin{cases} \sum_{cgC} \sum_{mgO_n} \sum_{keK_n} F^m_{cnk} & \text{flowrate capacity of unit n} \\ W_n & \text{work load of unit n} \end{cases} \qquad (12)$$

and they can be bounded by minimum and maximum capacities with the constraint

$$G^L_n \left(\sum_{k \in K_n} y_{nk}\right) \leq G_n \leq G^u_n \left(\sum_{k \in K_n} y_{nk}\right) \qquad (13)$$

Clearly logical constraints can also be added to indicate that for instance only one type of unit be selected among several possible choices. Finally, if the basic criterion in the synthesis is profit maximization, the objective functions will involve sales and purchases of chemicals, and linear investment cost of the units with fixed cost charges.

The constraint set given by the equalities and inequalities in (1) to (13) can be used to represent the superstructure of the chemical plant. However, as

formulated above, the transshipment model (P3) [10] for heat recovery networks would also have to be incorporated. As for the addition of the MILP model for utility systems, this can be done simply by treating the utility demands as variables, as for example the power W_n that is required by a given unit. In this way the MILP models of the chemical plant and utility system, as well as the LP transshipment model for heat recovery networks can be combined so as to yield an integrated MILP model for the total processing system.

Example Problem

In order to show the application of the synthesis strategy for total processing systems the following example 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, with the composition given in Table 1. 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 catalysts 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.

In order to apply the MILP approach for total processing systems, the operating conditions given in Table 1 are selected. Note that four different values are selected for the purge rate. Therefore, with the four options in the reactor and

the four options in the distillation sequence, 64 alternative flowsheets for the chemical plant will have to be analyzed.

The superstructure of the chemical plant is derived from the data given in Table 1, and is shown with its alternative processing steps in Fig. 2. 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 reactors having different catalysts, and for each reactor a medium (40 bar) or high (100 bar) pressure can be selected. Because the conversions per pass in the reactors are low (10 to 25%; see Table 1), 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 essentially 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, and part of it 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 possibe 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_f whereas the second column operates at 5 bar.

As it can be seen from the problem data given in Table 1, there are several discrete operating conditions considered for certain plant units of the proposed superstructure. The usual rule for selecting the plant units and the discrete conditions to be analyzed, is that only parameters that would affect significantly the performance of the units are considered. For example, the reactor pressure and catalyst are major parameters affecting the reactor conversion, recycle flowrate, heat loads in the streams, and the overall economics of the process. The same applies for the purge rate of the recycle stream, and the operating pressure of the distillation columns that can alter the temperature and heat loads in the corresponding condensers and reboilers. On the other hand, the absorber temperature is set to 310°K,where the mass transfer between products D, E and solvent W is most favorable, while the same pressure as in the reactor is used in the absorber to reduce the compression cost in the recycle.

In order to formulate the MTLP 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 modeling the reactors, flash, absorber and distillation columns as outlined by Westerberg [15], and using the data in Tables 1 and 2. The cost data of the chemicals is given in Table 3, and the fixed-charge cost correlations for investment cost were derived from Guthrie [1] and updated with the Chemical Engineering Index to 1981 prices. The heat recovery network corresponding to all process streams and utilities for this example is modeled using the transshipment model (P3) for minimum utility cost [10]. 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 HELP model presented in Papoulias and Grossmann [9] 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 turbine exhaust, and the cost data were the same as the values considered in the example problem of Papoulias and Grossmann [9].

Numerical results

The MILP model for the total processing system is obtained by adding the MILP synthesis models for the chemical plant and utility system, as well as the transshipment model (P3) for the heat recovery network. 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 [11] 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 $9,695,248/year.

The optimal configuration and operating conditions for the chemical processing plant are shown in Fig. 3. 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 reactor with the cheaper catalyst 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 recycled to the reactor after being recompressed. The optimal sequence of distillation columns necessary for product purification is the direct sequence at the lover pressure. The first column operates at 6 bar and separates the most volatile product D from components E and W, while the second column operates at 5 bar and separates by-product E from solvent W that is recycled back to the absorber.

The hot and cold process streams are shown on the flowsheet of Fig. 3 with circles that indicate the type (H=hot, C=cold) and the number of the stream. The optimal transshipment network (P3) 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. 4. 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 utilities 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 (P2) 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 [11] 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. 5. Note that this network does not require any stream splitting and contains one cycle (H1-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. 6. 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 Rankine 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 (261 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 above solution of the integrated MILP model for total processing systems, the option that was explored is to solve first the chemical plant and recovery network with nominal prices for the utilities, (see Table 4) and then synthesize the utility system at a second stage. The first formulation that is derived is the MILP synthesis model for the chemical plant augmented with the transshipment model (P3) for the heat recovery network. In order to account for the utilities in this model, the unit costs shown in Table 4 were assigned for each utility type. This MILP model involved 14 binary variables, 162 continuous variables, 120 rows and was solved using LINDO in approximately 1.6 minutes on a DEC-20 computer. The objective function for this formulation was to maximize the annual profit, and the value found at the optimal solution was $11,302,550/year. The fact that this value is larger than the $9,695,248/year obtained in the previous case is a clear indication that the utility prices

in Table 4 have been underestimated. However, the optimal configuration for the chemical plant is identical to the one obtained in Fig. 3, except that the optimal transshipment network is slightly different since now 305.4 Ton/hr of LP steam are used as the only heating utility. The reason for this difference is that the LP steam had a smaller unit cost than MP steam, and consequently was preferred at the optimal solution. It should be noted that the total heating requirement (heat load) is the same as the heat load provided by MP and LP steam in Fig. 4. Therefore, since the same heating requirements are obtained with both methods, the only alteration for the network structure shown in Fig 5 is in the elimination of the MP steam heater for (C4).

The design of the total system, is completed by synthesizing the utility system satisfying the demands determined at the optimal solution of the chemical processing plant and supporting heat recovery network. The utility demands for the chemical plant are 16050 kW of electricity, 11837 kW power to drive the feed compressor, 4369 kW power to drive the recycle recompressor, 1690 kW for the cooling water pump and 261 kW power for the solvent recycle pump in the absorber. The utilities required in the heat recovery network are 305.4 Ton/hr of LP steam for heating and 6487 Ton/hr water for cooling. The MILP synthesis model for this utility system has 20 binary variables, 120 continuous variables, 80 rows, and was solved with LINDO in approximately 1 minute on a DEC-20 computer. The value of the objective function corresponding to the minimum annual cost for this optimal design was $29,453,307/year, and is identical to the utility system obtained with method 1 (Fig. 6), except that the 53.7 Tons/hr of MP steam are reduced to low pressure with water addition and combined with the 242.4 Tons/hr of LP steam to provide the 305.4 Tons/hr of LP steam required for heating in the heat exchanger network. Therefore, it is apparent that there is some weakness involved in the proposed decomposition, since synthesizing separately the chemical plant with the supporting heat recovery

network can determine utility demands that are not provided most efficiently by the utility system. Also, note that the computer requirements in the decomposition scheme were only slightly smaller when compared to the time required for solving the MILP for the total processing system.

Discussion

As was demonstrated with the example problem, the synthesis models presented in the two previous papers [9], [10] are compatible with the MILP model for the chemical plant. It was shown that these models can easily be connected for the simultaneous synthesis of total processing systems. With this approach the interactions among the chemical plant, heat recovery network and utility plant can be accounted in a rigorous and natural way. It is considered that it is this feature that makes the proposed synthesis strategy truly original, as other previous methods reported in the literature cannot accomplish this objective.

A point that should be apparent from the example is that the MILP approach 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 so as to find those solutions whose cost lies within a given percentage of the optimal value.

Finally, the example solved in this paper has shown that the MILP approach for process synthesis does not preclude the use of heuristics or thermodynamic targets. This was illustrated with the heat recovery network in which the objectives of minimum utility cost and minimum number of units were incorporated into the model. It is clear that these objectives made the MILP of the example problem easier to solve. On the other hand, it is doubtful that if one were to use only heuristics and thermodynamic targets that one would have been able to obtain the optimal solution of the example problem as readily as with the MILP model. Therefore, it would seem that it is a balanced combination of heuristics, thermodynamic targets and mixed-integer programming that is needed to solve effectively the problems in process synthesis.

Acknowledgement

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Table 1. Stream/Equipment Cdnditions For Example Problem

STREAM/EQUIPMENT	CONDITIONS
FEED	
Conditions	P = 16 bar, T = 320 K
Component A	Mole Fraction = 0.40
Component B	Mole Fraction = 0.45
Component C	Mole Fraction = 0.15
REACTOR	
Chemical Reaction:	A + B -~* D + E
Heat of Reaction (40bar)	ΔH_{rxn} = 41,860 kj/kg-mole
Heat of Reaction (lOObar)	ΔH_{rxn} = 50,240 kj/kg-mole
Operating Conditions:	
Catalyst Cl	p = 40 bar, T = 550 K, Conversion =0.10
Catalyst C2	p = 40 bar, T = 550 K, Conversion =0.16
Catalyst Cl	p = 100 bar, T = 600 K, Conversion =0.18
Catalyst C2	p = 100 bar, T = 600 K, Conversion = 0.25
ABSORBER	
Operating Condition	P = 40 or 100 bar, T=310 K
Solvent W	
Recovery	Recovery of Key Component D = 99%
FLASH	
Operating Condition	P = 40 or 100 bar, T=310 K
Recovery	Recovery of Key Component D = 0.26
SPLITTER	
Purge Rates Considered	0.5% , 2% , 5% , 10%
DISTILLATION COLUMNS	
Column (D/EW)	
Operating Condition	P = 20 bar, Recovery of Keys » 0.98
Operating Condition	P =
Column (E/W)	6 bar, Recovery of Keys = 0.98
Operating Condition	P =
Column (DE/W)	5 bar, Recovery of Keys =0.98
Operating Condition	P =
Operating Condition	P = 20 bar, Recovery of Keys =0.98
Column (D/E)	6 bar, Recovery of Keys =0.98
Operating Condition	P = 5 bar, Recovery of Keys = 0.98
COMPRESSORS	
Feed Compressor:	
Outlet Pressure	P = 40 bar, Compression Ratio = 2.5 (1 stage)
Outlet Pressure	P = 100 bar, Compression Ratio = 2.5 (2 stages)
Recycle Recompressor:	
Outlet Pressure	P = 40 bar, Compression Ratio = 1.04
Outlet Pressure	P = 100 bar, Compression Ratio = 1.04

Table 2. Physical Properties of Components in Example Problem

	Components					
	A	B	C	D	E	W
Molecular weight	44	50	67	32	62	18
C_p(kj/kg o_K)	0.9	1.0	1.2	1.1	1.4	4.18
AH_{vap}(kj/kg)	390	468	672	1047	1302	2326
Normal boiling point (°K)	194.7	168	206.8	325	353	373
Antoine's coefficients						
ANTA	22.5898	20.233	19.3624	13.9	12.8766	11.3351
ANTB	3103.39	2327.94	1606.37	2932.45	2348.98	1528.3
ANTC	-0.16	3.19	-80.59	79.26	23.99	-48.39

Antoine's equation $\ln VP = ANTA - \frac{ANTB}{ANTC + T}$, VP ($mm H_g$), T (°K)

Compressors: $Y = (^{c}_{p}/^{c}v) = 1.4$

Abosrber: Absorption factor of D = 1.4

Table 3: Economic Data for Example Problem

Annual Operation	8400 hrs.
Capital Recovery Factor	0.154252
FEED	Cost =0.10 $/kg
PRODUCTS	
Main Product D	Price = 0.28 $/kg
Byproduct E	Price =0.12 $/kg
BLEED	Credit « 0.06 $/kg
CATALYST	
Catalyst Cl	Cost = [2.0 * reactor feed(kg/hr)3 $\frac{\$}{yr}$
Catalyst C2	Cost = [4.0 * reactor feed(kg/hr] $\frac{\$}{yr}$
UTILITES	
Gas Turbine Fuel	Cost = 143 $/Ton
Fired Boiler Fuel	Cost =114 $/Ton
Water	Cost = 0.05 $/1000 gal,
HEAT EXCHANGERS	Cost = 2 $/kW

Table 4. Nominal Prices for Utilities

Electricity (includes generator)	0.40 $/kwh
HP Steam	6.5 $/Ton
MP Steam	5.4 $/Ton
LP Steam	4.0 $/Ton

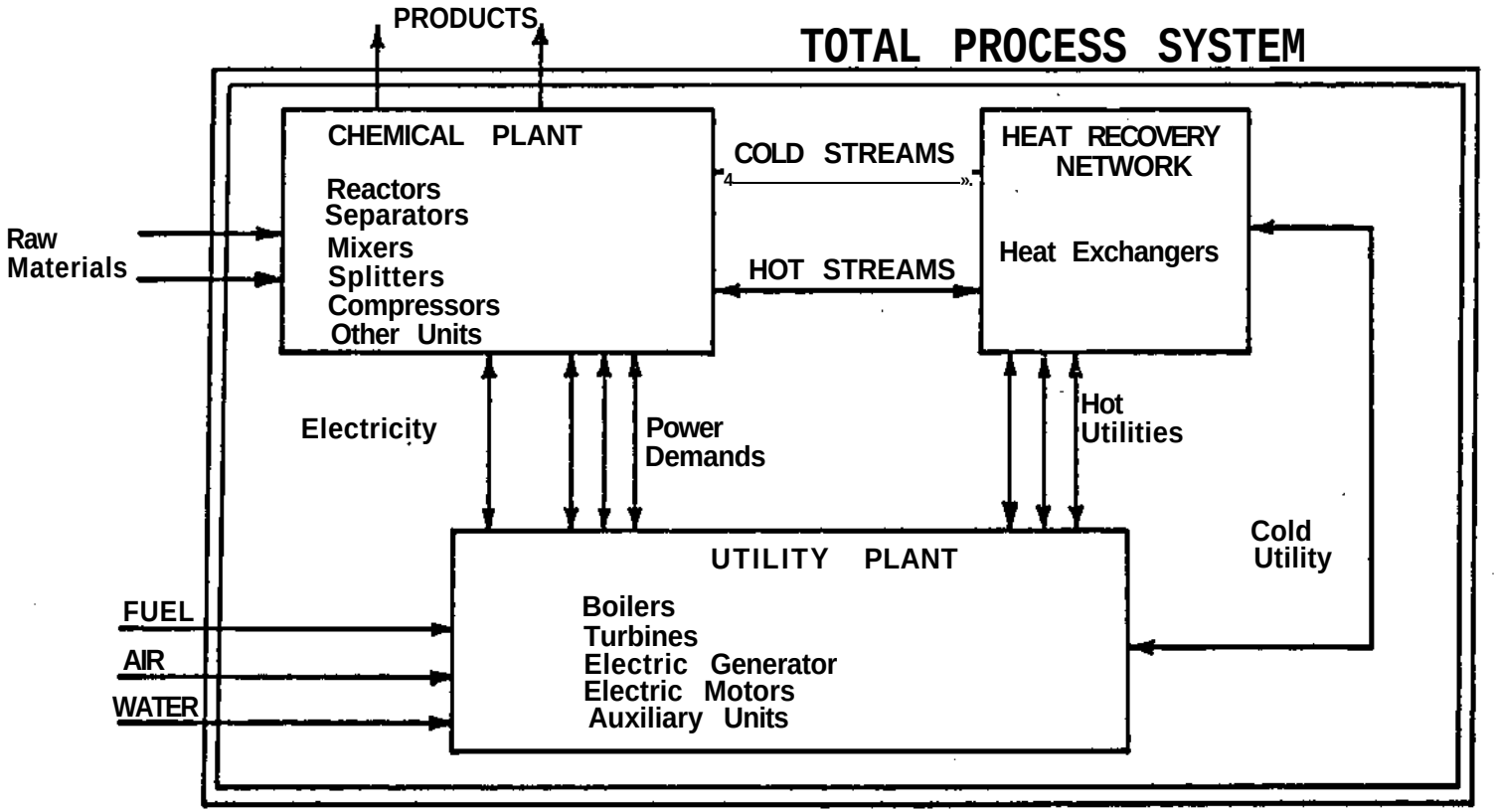

PRODUCTS
TOTAL PROCESS SYSTEM
CHEMICAL PLANT
Reactors
Separators
Mixers
Splitters
Compressors
Other Units
COLD STREAMS
HOT STREAMS
HEAT RECOVERY NETWORK
Heat Exchangers
Raw Materials
Electricity
Power Demands
Hot Utilities
Cold Utility
UTILITY PLANT
Boilers
Turbines
Electric Generator
Electric Motors
Auxiliary Units
FUEL
AIR
WATER

Fig. 1

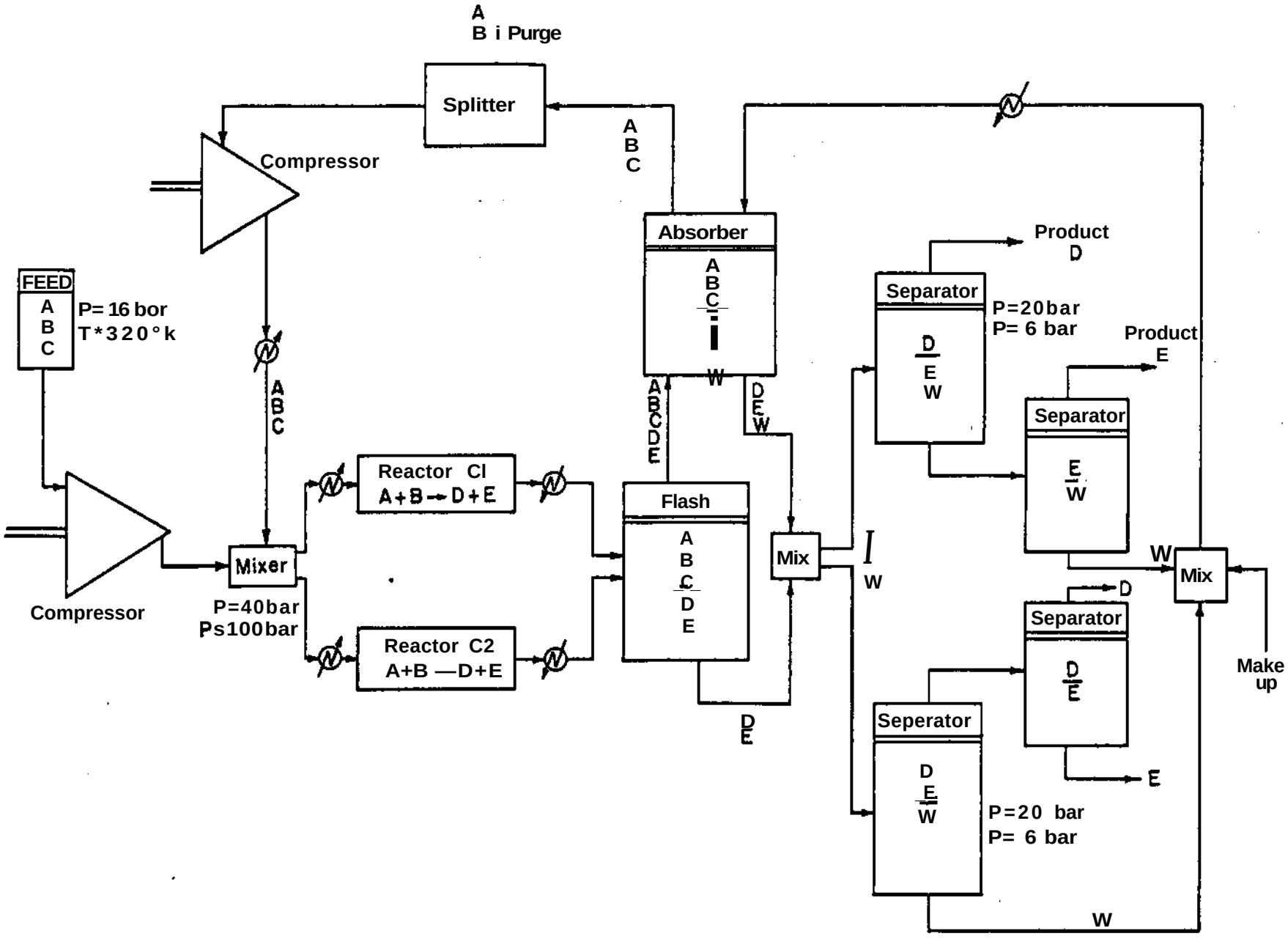
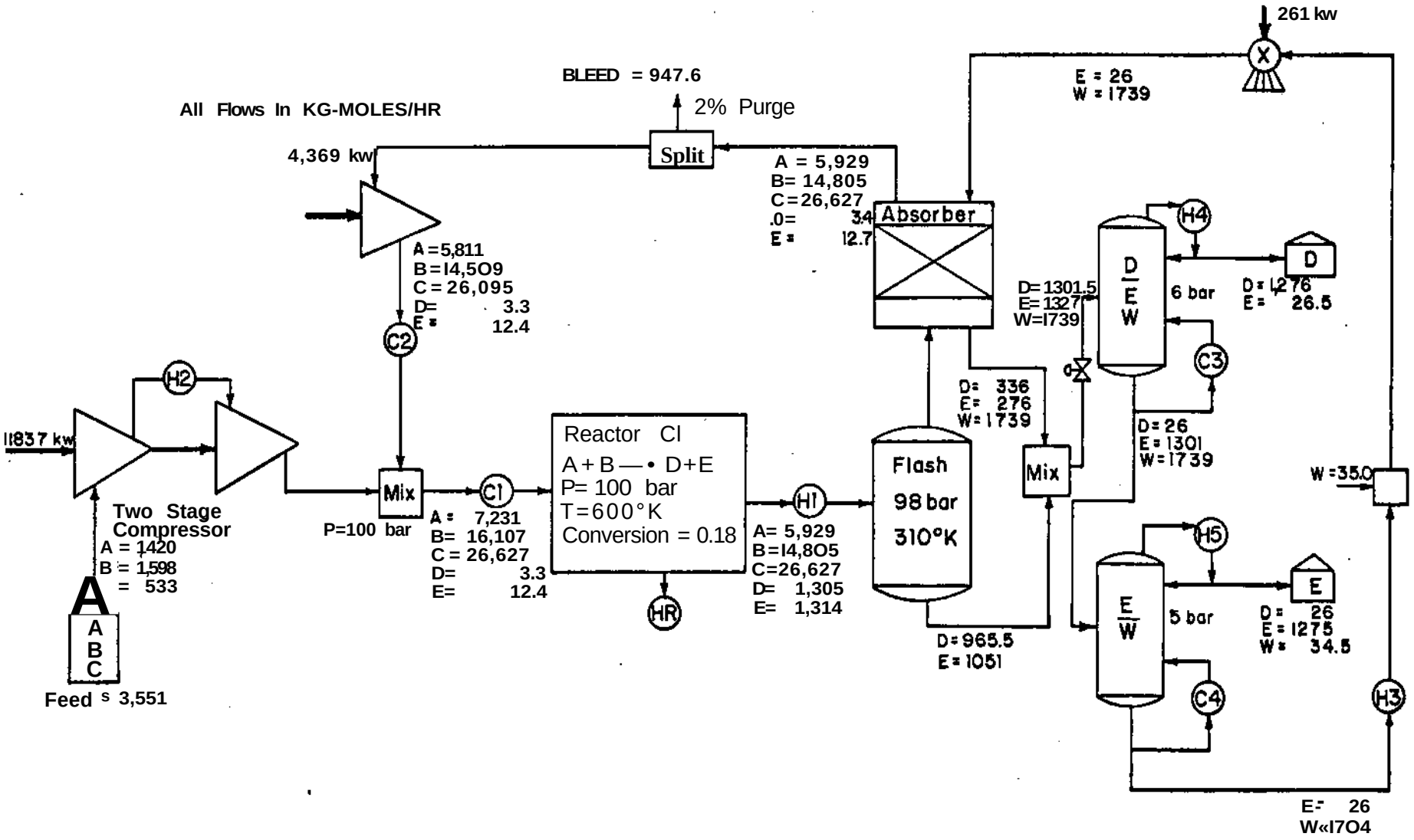

A
B i Purge
Splitter
Compressor
A
B
C
Absorber
A
B
C
W
Product
D
Separator
D
E
W
P=20bar
P= 6 bar
Product
E
Separator
E
W
FEED
A
B
C
P= 16 bor
T*320°k
A
B
C
Reactor Cl
A+B D+E
Flash
A
B
C
D
E
Mix
W
Mix
W
Separator
D
E
Make
up
Compressor
Mixer
P=40bar
Ps100bar
Reactor C2
A+B —D+E
D
E
Seperator
D
E
W
P=20 bar
P= 6 bar
E
W

Fig. 2


All Flows In KG-MOLES/HR
BLEED = 947.6
2% Purge
Split
261 kw
E = 26
W = 1739
4,369 kw
A = 5,929
B= 14,805
C=26,627
.0= 3.4
E = 12.7
Absorber
A=5,811
B=14,509
C = 26,095
D= 3.3
E = 12.4
C2
H2
11837 kw
Two Stage
Compressor
A = 1,420
B = 1,598
= 533
A
A
B
C
Feed s 3,551
Mix
P=100 bar
C1
A = 7,231
B= 16,107
C = 26,627
D= 3.3
E= 12.4
Reactor Cl
A + B — • D+E
P= 100 bar
T=600°K
Conversion = 0.18
HR
H1
A= 5,929
B=14,805
C=26,627
D= 1,305
E= 1,314
Flash
98 bar
310°K
D= 336
E= 276
W= 1739
D= 965.5
E= 1051
Mix
D= 1301.5
E= 1327
W=1739
D
E
W
6 bar
H4
D = 1,276
E = 26.5
C3
D= 26
E = 1301
W=1739
W =35.0
H5
E
W
5 bar
D = 26
E = 1275
W = 34.5
C4
H3
E= 26
W«17O4

Fig, 3

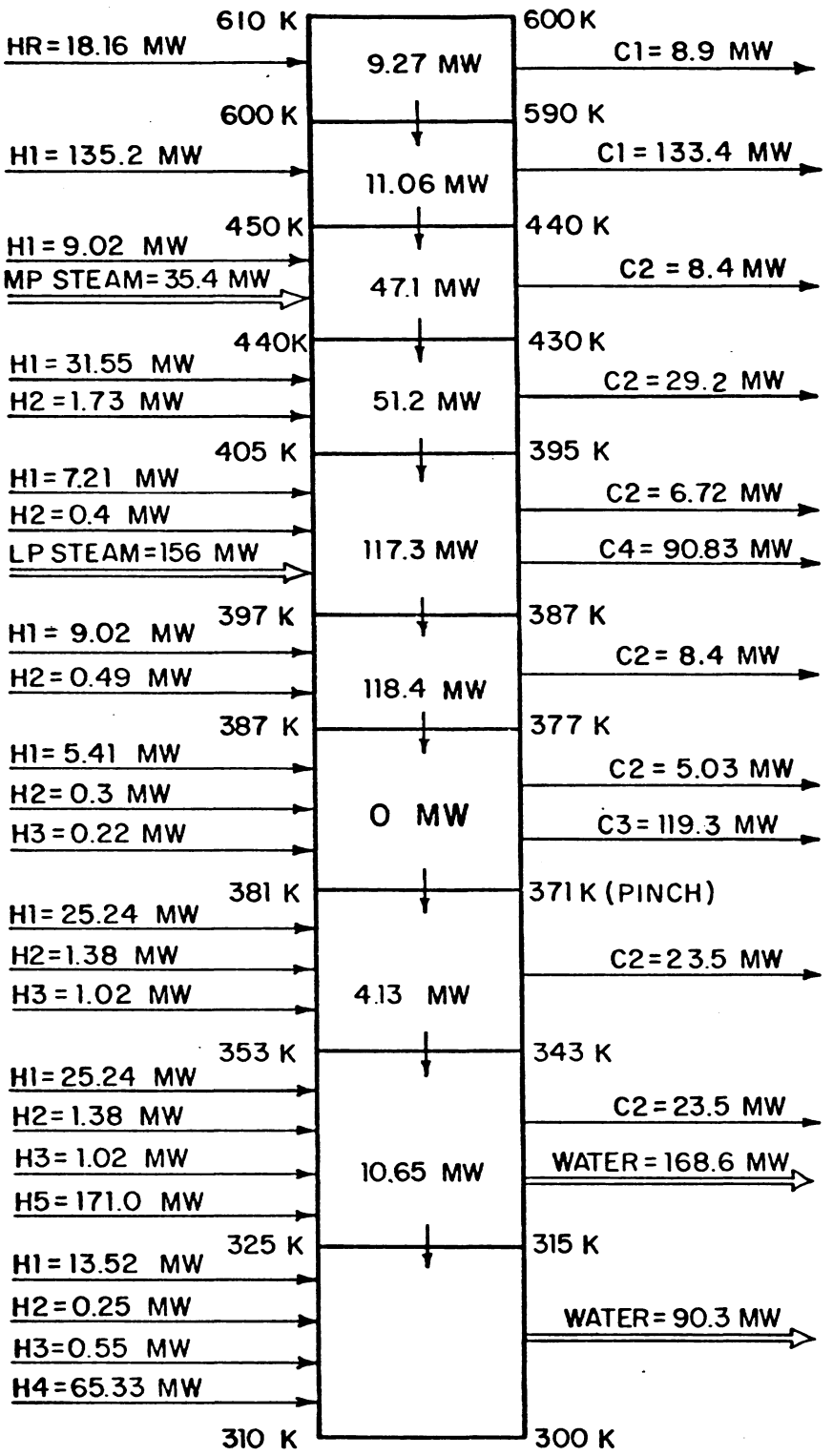

610 K
HR = 18.16 MW
600 K
9.27 MW
600 K
C1 = 8.9 MW
600 K
590 K
H1 = 135.2 MW
11.06 MW
C1 = 133.4 MW
450 K
440 K
H1 = 9.02 MW
MP STEAM = 35.4 MW
47.1 MW
C2 = 8.4 MW
440K
430 K
H1 = 31.55 MW
H2 = 1.73 MW
51.2 MW
C2 = 29.2 MW
405 K
395 K
H1 = 7.21 MW
H2 = 0.4 MW
LP STEAM = 156 MW
117.3 MW
C2 = 6.72 MW
C4 = 90.83 MW
397 K
387 K
H1 = 9.02 MW
H2 = 0.49 MW
118.4 MW
C2 = 8.4 MW
387 K
377 K
H1 = 5.41 MW
H2 = 0.3 MW
H3 = 0.22 MW
0 MW
C2 = 5.03 MW
C3 = 119.3 MW
381 K
371 K (PINCH)
H1 = 25.24 MW
H2 = 1.38 MW
H3 = 1.02 MW
4.13 MW
C2 = 23.5 MW
353 K
343 K
H1 = 25.24 MW
H2 = 1.38 MW
H3 = 1.02 MW
H5 = 171.0 MW
10.65 MW
C2 = 23.5 MW
WATER = 168.6 MW
325 K
315 K
H1 = 13.52 MW
H2 = 0.25 MW
H3 = 0.55 MW
H4 = 65.33 MW
WATER = 90.3 MW
310 K
300 K

Fig. 4

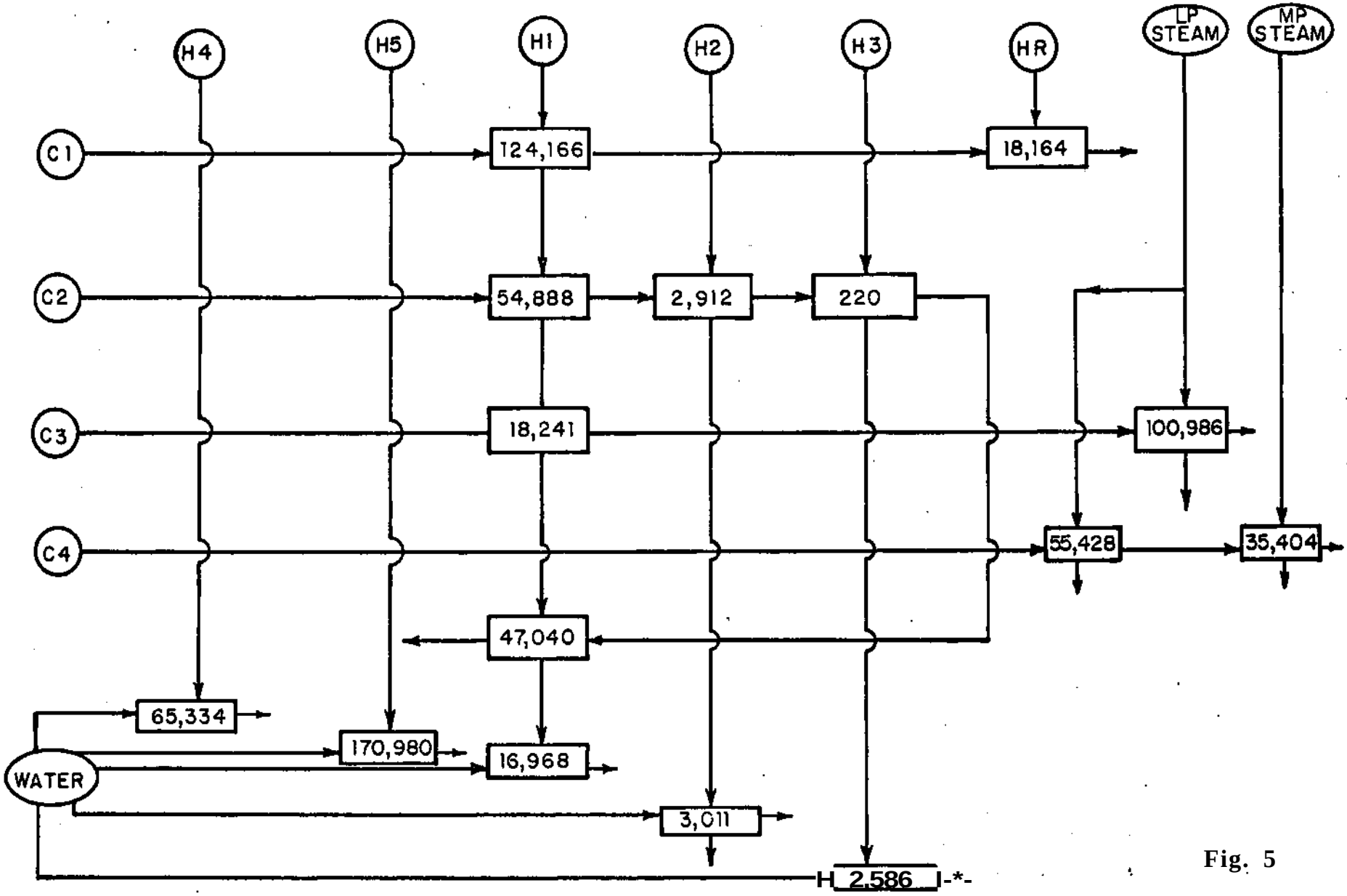

H4
H5
H1
H2
H3
HR
LP STEAM
MP STEAM
C1
C2
C3
C4
124,166
18,164
54,888
2,912
220
18,241
100,986
55,428
35,404
47,040
65,334
170,980
16,968
WATER
3,011
2,586

Fig. 5

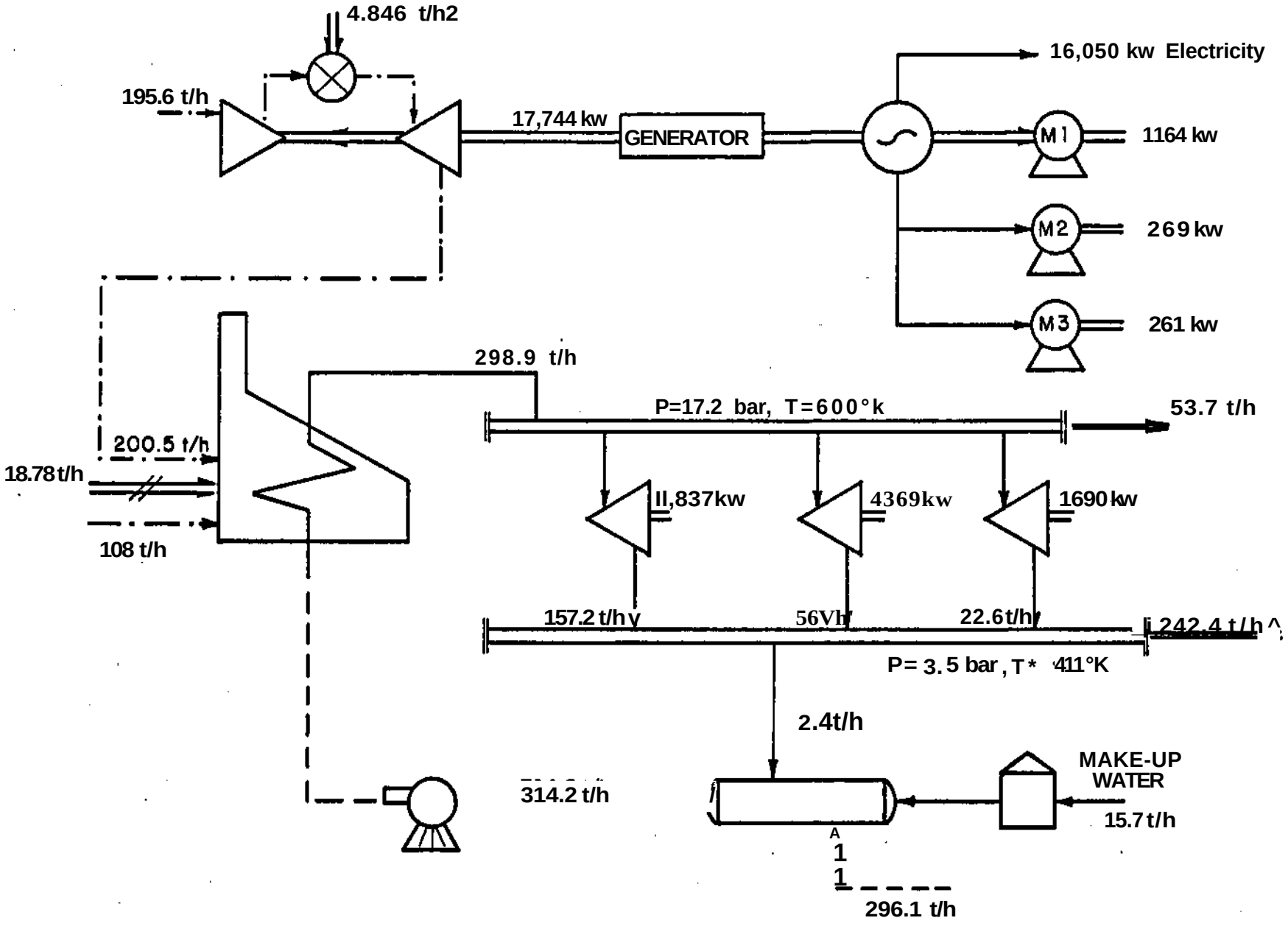

4.846 t/h2
195.6 t/h
17,744 kw
GENERATOR
16,050 kw Electricity
M1
1164 kw
M2
269 kw
M3
261 kw
298.9 t/h
P=17.2 bar, T=600°k
53.7 t/h
200.5 t/h
18.78t/h
108 t/h
ll,837kw
4369kw
1690kw
157.2 t/h
56Vh
22.6t/h
242.4 t/h
P= 3.5 bar, T* 411°K
2.4t/h
314.2 t/h
MAKE-UP
WATER
15.7t/h
A
296.1 t/h

Fig. 6