**Simultaneous Optimization Models
For   Heat   Integration-III**

by

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SIMULTANEOUS OPTIMIZATION MODELS FOR HEAT INTEGRATION--III

Process and Heat Exchanger Network Optimization

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ABSTRACT

In this paper, the proposed heat integration representation of Part I (Yee et aL, 1990) is used for the *simultaneous* optimization or synthesis of the process and its heat exchanger network. The basic idea involves embedding the proposed representation into a given process flowsheet or superstructure and optimize the combined superstructure simultaneously, where flows and temperatures of the potential heat integrated streams are treated as variables. The proposed model accounts for capital and operating costs of the heat exchanger network. It does not require the specification of a heat recovery approach temperature (HRAT) and can easily handle constraints for heat integration. Examples are presented to Illustrate the capabflities of the simultaneous model which can be formulated as an NLP problem or as an MINLP problem when the structure of the network is to be determined explicitly.

INTRODUCTION

In the synthesis of a process, the heat exchanger network (HEN) is usually designed *after* the process flowsheet has been optimized. Such a sequential procedure is discussed in Unnhoff and Townsend (1981) and Douglas (1985). As shown in Figure 1, the sequential approach follows the progression that the process without heat integration must be designed first in order to establish values for stream flow rates and temperatures which are needed by the current methods to design the HEN. The limitation of this approach, however, lies in the fact that there exists a strong interaction between the process and the potential heat integration. Changes in the process parameters can lead to values of *fixe* stream flow rates and temperatures which can have great impact on the process flowsheet as well as on the amount of heat integration which can significantly change the utility requirement for the system. In addition, the variations can greatly affect the possfole driving forces for the heat exchanger network which can significantly change its capital cost requirement In general, a sequential scheme cannot properly account for the trade-off between the capital cost of the process, the capital cost for the HEN, and the utility cost for both the process and the HEN.

ideally, the process and the HEN should be designed simultaneously as shown in Figure 2, where **flows and** temperatures are optimized accounting for both the process and the HEN. Although no paper has explicitly addressed this problem, several papers have proposed procedures for simultaneous optimization and heat integration of processes where the flowsheet optimization is performed so to satisfy the minimum utility cost target for a given heat recovery approach temperature (HRAT). The level of heat recovery determined from this problem is then used to synthesize the detailed structure of the HEN.

Papouiias and Grossmann (1983) first proposed a strategy for simultaneous optimization and heat integration based on mixed integer linear programming where the LP transshipment model is embedded into the process formulation to account for the maximum possible heat integration and its utility consumption. While flows can be treated as continuous variables, temperatures in the model can only assume a given set of prespecified values. As a result, the effectiveness of the optimization depends greatly on the prespecified temperatures given. Duran and Grossmann (1986) overcame this limitation by formulating a nonlinear programming model, which through the use of special inequality constraints that involve max operators can predict the minimum utility requirements for variable flows and temperatures of the process streams and for a fixed value of HRAT. Based on the Duran and Grossmann model, Lang et aL, (1988) developed a formulation for use with sequential modular simulators. Their results on an

ammonia and methanol process show that the overall raw material conversion in a process will increase when heat integration is simultaneously considered with the process optimization leading to higher profits. The limitations of all these methods, though, are that they all require the specification of a heat recovery approach temperature (HRAT) and that they do not consider the heat exchanger network capital cost.

Viswanathan and Evans (1989) more recently presented two models for the problem. The first, the fixed TI-grid method uses temperature intervals which are determined by a set of rules. These intervals do not necessarily correspond to the supply and target temperatures of the streams and can lead to an overestimation of the possible heat integration. The second method uses the concept of variable temperature intervals. The intervals are set up according to a representation which is similar to the one described in Part I (Yee et al., 1990) of this series of paper. However, the mathematical model is significantly different since nonlinear flow variables are used to represent stream splits and a nonlinear heat balance is performed at each potential exchanger. Furthermore, in this formulation, the capital cost of the HEN is not considered.

Kravanja and Grossmann (1989) have recently proposed a step-wise procedure for simultaneous optimization and heat integration that does account for the cost of area assuming vertical heat transfer. In the outer loop, the relative ordering of temperatures in the composite curves is determined to calculate the temperature driving forces. In the inner loop, the NLP optimization is solved calculating the area for the given ordering of temperatures. If this ordering is maintained, the procedure stops; otherwise, if a new order is obtained, the NLP is resolved. It should be noted that this method cannot handle constraints and only approximates the area requirements for the actual network.

In this paper, the heat integration representation proposed in Part I (Yee et al., 1990) will be embedded in a process flowsheet or superstructure in order to perform the simultaneous optimization or synthesis of the HEN and process. As will be shown, the heat integration can be incorporated into the process model by a set of NLP constraints or MINLP constraints if the structure of the network is to be determined explicitly. Based on the constraints that have been presented in Part I (Yee et al., 1990) for the simultaneous targeting of energy and area for HEN and in Part II (Yee and Grossmann, 1990) for the synthesis of HEN, constraints are extended so that temperatures and flow rates of the streams can be treated as variables for the optimization of the process flowsheet and HEN. The optimization explicitly accounts for the trade-offs between capital cost and operating cost for the process flowsheet and the capital cost and the utility cost for the HEN. No specification of a minimum approach temperature (HRAT)

is required and constraints for matches can be easily handled. The application of this combined general mathematical model for the simultaneous optimal design of HEN and processes will be illustrated with two example problems.

PROBLEM STATEMENT

The problem of simultaneous synthesis or optimization of a process flowsheet with the HEN can be stated as follows. Given are:

« Process flowsheet or a superstructure embedding alternative process flowsheets and the corresponding equations of heat and material balances and design constraints.

• Streams in the flowsheet which are to be heat integrated:

1. Set of N_H hot process streams *HP to* be cooled.

2. Set of y^coid process streams *CP* to be heated.

3. Set of hot utilities *HU* and cold utilities *CU* and their corresponding inlet and outlet temperatures.

The objective is then to determine:

• Optimal process flowsheet and design parameters.

• Values for stream flow rates and temperatures for the process and heat exchanger network.

• Optimal HEN configuration including values for area, number of units and utility requirement.

Like the models presented in the other papers of this series, assumptions for the HEN design include the following:

• Constant heat capacities

• Constant heat transfer coefficients

« Countercurrent heat exchangers

• Each match corresponds to a one shell exchanger

Also, for the sake of simplicity, it will be assumed that only one hot and one cold utility are available. This assumption can be easily relaxed to account for multiple utilities with different temperatures and costs. In addition, the superstructure or flowsheet for the given process *without heat integration* is assumed to be modeled by the formulation below which follows the presentation given in Ouran and Grossmann (1986):

$$\min \quad \ast = F(w,s) + \sum_{y \in CP} CCU\, qcu_i + \sum_{i \in /\!/\!/>} CHU\, qhu_j$$

s.t $A(HM) = 0$

$g(w,x) \prec 0$

$qcu_i = r_i(x), \quad i \in HP$

qhu'

$qcu_{i\%}\ qhuj\ Z\ 0, \quad i \in HP,\ je\ CP$ (P0)

Note that the process parameters are divided into two sets, *weW* and *xeX*. The variables *x* represent the process parameters which are involved with the potential heat integration such as hot and cold stream flow rates *{f₁ and jrⱼ)* and stream supply and target temperatures *(tin_{i9} tin^ tout_{i\%} tout}*. The variables *w* represent the remaining parameters such as pressures, temperatures, equipment sizes, or even structural parameters (0-1 variables) which are needed to define the process flowsheet

Constraints *h* and *g* correspond to the set of process constraints such as material and energy balances, specifications for design, and any logical constraints if 0-1 variables are used. Also, the functions *rfic)* and *rfic)* determine the amount of heating and cooling utilities required for each of the hot and cold streams, respectively. Note that in the objective function, these utility requirements are explicitly accounted since no heat integration is performed. Besides these utility costs, the function *F&w)* also appears in the objective function to represent the capital and other operating costs for the process.

STRATEGY

The proposed method for simultaneous process and HEN synthesis makes use of the superstructure representation developed in Part I (Yee et aL, 1990) of this series of papers to account for the potential heat integration and to design the HEN. The basic idea is to embed the representation into the given superstructure or flowsheet of the process. This can be done easily by first determining the potential streams in the process superstructure or flowsheet which are to be heat integrated. These streams then represent the potential hot and cold streams for the HEN and thus are used to construct the heat integration representation. An example of a combined process and heat integration representation is shown in Figure 3. For the given process flowsheet or superstructure, the potential streams for heat integration are hot streams H1 and H2 and cold streams C1 and C2. Since maxfA^, A'ᶜ}=2, a two stage representation for heat integration is used. Unlike the models presented in Part I (Yee et a!., 1990) and Part II (Yee and Grossmann, 1990), however, the stream flow rates (/) and supply and target

temperatures *(ṅin, tout) are* not necessarily fixed parameters. Frequently, these parameters are variables **to be optimized for** the **process superstructure or flowsheet As** a result, they must **be treated** as **optimization variables** *in* **order to account for the** trade-offs **in both** the process flowsheet and in the HEN.

Given the models in Part I (Yee et al., 1990) and II (Yee and Grossmann, **1990),** there exists the **option of either using an NLP formulation to design the HEN or an MINLP formulation where structural considerations and fixed charges for units can be explicitly accounted for through the binary variables. The advantage of using an NLP formulation is that binary variables and logical equations are not needed, which means that the computational time required will often be smaller. The advantage of the MINLP-formulation is that it can more accurately account for the cost of the HEN, it does not require the use of smooth approximations for the max operators, and it enables more control over the structural aspects of the HEN design through constraints involving binary variables. Furthermore, the solution of the MINLP model provides directly the structure of the optimal HEN. The solution of the NLP formulation will tend to yield only an approximation of the network structure since it cannot treat fixed cost charges.**

In general, one can select which heat integration model to *use* **by following the type of process model to be optimized. If the formulation for the process does not require binary variables, such as the optimization of a fixed flowsheet one would probably use the NLP model, while if the process model does require binary variables, one would probably use the MINLP model. In this way, one does not change the synthesis model type when heat integration is embedded into the process model.**

Since the proposed heat integration representation does not rely on the definition of temperature intervals, there is no need to check for feasfoifity according to the composite curves nor changes in the pinch point location. In addition, there is no need to specify values for HRAT or for the minimum approach temperature EMAT. Instead, the model optimizes these quantities to derive a design which minimizes annual operating and capital costs. Moreover, since the capital cost of the HEN can be explicitly considered, the optimization of the combined process and HEN superstructure accounts for all **the trade-offs of capital and utility costs for and between the** process and **HEN.**

Finally, the assumption **on** the **type of** stream splitting allowed which was used *in* the development of the models presented in Part I and Part II is once again used here. The assumption simply specifies that the outlet temperature of a particular stream at each exchanger of a stage is the same as the outlet temperature of the stage. The assumption simplifies the model greatly since stage temperatures can be

used to calculate area requirement of the exchangers and as a result, many nonlinear and nonconvex expressions and constraints can be eliminated.

In the next section, the formulation for the combined process and HEN model is presented. The formulation is given for both the NLP and the MINLP cases. The presentation will take into account the assumptions for stream splitting as discussed above and the fact that only one hot and one cold utility are available for heating and cooling the process streams with utility exchangers placed at the outlet of the superstructure representation.

FORMULATION

In order to define the formulation for the simultaneous optimization or synthesis of the process and HEN, the following definitions are necessary:

(i) Indices

i = hot process or utility stream $\qquad$ j = cold process or utility stream

k = index for stage 1..NOK and temperature location 1..$NOK+1$

(ii) Sets

$HP = \{i|i$ is a hot process stream$\}$ $\qquad$ HU = hot utility

$CP = \{j|j$ is a cold process stream$\}$ $\qquad$ CU = cold utility

$ST = \{k|k$ is a stage in the superstructure, $k=1..NOK\}$

$W = \{w|w$ is a process variable not involved with heat integration$\}$

$X = \{x|x$ is a process variable involved with heat integration$\}$

(iii) Parameters

CCU = per unit cost for cold utility $\qquad$ CHU = per unit cost for hot utility

CF = fixed charge for exchangers $\qquad$ C = area cost coefficient

B = exponent for area cost $\qquad$ NOK = total number of stages

U = overall heat transfer coefficient

Ω = an upper bound for heat exchange $\qquad$ Γ = an upper bound for temperature difference

(iv) Variables

f = heat capacity flow rate

tin = inlet temperature of stream

tout = outlet temperature of stream ∴.:••--•-/^-z.V-W--•••>.•-...

dt_{iJk} m temperature approach for match *(ij)* at temperature location *

$dtcu$^ temperature approach for the match of hot stream *I* and cold utility ··

$dthu_j$ = temperature approach for the match of cold stream *j* and hot utility

q_{ijk} = heat exchanged between hot process stream *i* and cold process stream *y* in stage *k*

qcu_i« heat exchanged between hot stream i and cold utility

qku_j = heat exchanged between hot utility and cold stream *y*

l^ = temperature of hot stream i at inlet of stage *k*

fa «temperature of cold stream *y* at outlet of stage *k*

x = variable used to define process flowsheet or superstructure involved with heat integration

w • variable used to define process flowsheet or superstructure not involved with heat integration

z_{ijk} m binary variable to denote existence of match *(ij)* in stage *k*

icu_i «= binary variable to denote that cold utility exchanges heat with hot stream *I*

ihu_j -m binary variable to denote that hot utffity exchanges heat vwmcoW stream *y*

In the proposed formulation, constraints and objective function terms for the process are represented in a general form following the notations of formulation *(PO)* presented previously. The process contribution to the objective function is expressed by $F(w_jc)_{\%}$ which corresponds to a function for calculating the capital and operating cost for the process. The variables $x \in X$ are the process variables which are potentially involved with the heat integration such as ones defining the stream flow rates and temperatures $\{f_{i\%} \, l_{,} \, un_?, \, tin_{j}, \, tout^{,} \, tout_{j}\}$. The variables we *W* represent the rest of the process variables including potential 0-1 parameters which may be required for defining the structure of the process.

Constraints for the process are also represented in general form by the following equations:

$$K_w) = 0$$

$$g(*_s) < 0 \tag{1}$$

With these expressions and constraints, the flowsheet or superstructure lor tlie process is fully defined.

To account for the potential heat integration in the process model, constraints and expressions similar to the ones presented in Part I (Yee et al., 1990) for simultaneous energy and area targeting and Part II (Yee and Grossmann, 1990) for the synthesis of HEN are used. Note that the heat integration model can be incorporated into the process model with or without the use of binary variables, in the presentation below, the heat integration portion of the formulation is first presented as an NLP where no binary variables are used and then extended to the case where binary variables are used for modeling the structural decisions in the HEN. The explanation for the formulation is kept brief and the reader is referred to the other two parts (Yee et al., 1990, Yee and Grossmann, 1990) for a detailed discussion: Also, in the presentation below, the variables $x \in X$ are explicitly written out as f, *tin,* or *tout.*

Overall heat balance for each stream

An overall heat balance determines the total heat transfer required by each stream:

$$(tin_i - tout_i) f_i = \sum_{k \in ST} \sum_{j \in CP} q_{ijk} + qcu_i \qquad i \in HP$$

$$(tout_j - tin_j) f_j = \sum_{k \in ST} \sum_{i \in HP} q_{ijk} + qhu_j \qquad j \in CP \qquad (2)$$

Note that in the above equations, the left-hand side involves nonlinear terms since in general, f, *tin,* and *tout* are variables.

Heat balance at each stage

A heat balance for each stream at each stage determines the heat load for each exchanger represented in the superstructure:

$$(t_{i,k} - t_{i,k+1}) f_i = \sum_{j \in CP} \qquad k \in ST, \quad i \in HP$$

$$(t_{j,k} - t_{j,k+1}) f_j = \sum_{i \in HP} \qquad k \in ST, \quad j \in CP \qquad ()$$

In the above equations, note that the left-hand side also involves nonlinear terms.

Assignment of superstructure inlet temperatures

Inlet stream temperatures are assigned for the heat integration superstructure,

$$tin_i = t_{i,1} \qquad i \in HP$$

$$tin_j = t_{j,NOK+1} \qquad j \in CP \tag{4}$$

Feasibility of temperatures

A monotonic progression of temperature through the stages is defined such that stage *k=1* has *the* highest temperatures,

$$t_{i,k} \geq t_{i,k+1} \qquad k \in ST \quad i \in HP$$

$$t_{JJc} \ Z \ t_{jMI} \qquad k \in ST, \quad j \in CP$$

$$tout_i \leq t_{i,NOK+1} \qquad \_ \ P \tag{5}$$

$$tout_j \geq t_{j,1} \qquad j \in CP$$

Note that the slack in the last two inequalities of (5) corresponds to the temperature difference that is to be cooled and heated by utilities respectively.

Hot and cold utility load

Utility requirement for each stream is calculated by a heat balance using the required outlet temperature of each stream and the stream's last stage temperature:

$$(\ _{<WOIM} - tout_i \ ) f_i = qcu_i \qquad i \in HP$$

$$(\ toutj - t_{jk} \ ) fj = qhuj \qquad j \in CP \tag{6}$$

which in general correspond to nonlinear equations.

As compared to the constraints for the formulations presented in the earlier papers of this series, the primary difference of the above constraints is that the stream flow rates and temperatures are variables since they correspond to variables that are to be optimized for the process. However, in certain cases, depending on the process flowsheet or superstructure, some of these variables may actually be fixed values. For these cases, the variables can either be substituted by the fixed values directly in the formulation or {he variables can be properly bounded to the fixed values. For simplicity, though, all the

flows and temperatures has been presented as variables to reflect the general case.

In the objective function, the costs include that of the process flowsheet, $F(w,x)$, and the utility and capital cost required by the HEN. For an NLP formulation, the cost expressions for the HEN are the same as the ones presented for the simultaneous energy and area targeting model of Part I (Yee et al., 1990). These cost expressions do not explicitly account for the fixed charges for heat exchanger units. With a fractional cost exponent B in the objective function, though, the economy of scale for the area cost are accounted for. The combined objective function for both the process and the HEN are then as follows:

$$
\begin{aligned}
MIN \quad & F(w,x) + CCU \sum_{i \in HP} qcu_i + CHU \sum_{j \in CP} qhu_j + \\
& C_{ij} \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} [q_{ijk} / (U_{ij} \, LMTD_{ijk})]^{B_{ij}} + \\
& C_{i,CU} \sum_{i \in HP} [qcu_i / (U_{i,CU} \, LMTD_{i,CU})]^{B_{i,CU}} + \\
& C_{HU,j} \sum_{j \in CP} [qhu_j / (U_{HU,j} \, LMTD_{HU,j})]^{B_{HU,j}}
\end{aligned}
\tag{7}
$$

where the Chen approximation (1987) can be used to define the $LMTD$ terms:

$$
LMTD_{ijk} = [max(0, t_{ik}-t_{jk}) \; max(0, t_{ik+1}-t_{jk+1}) \; \{max(0, t_{ik}-t_{jk}) + max(0, t_{ik+1}-t_{jk+1})\}/2]^{1/3} + \delta
\tag{8}
$$

$$
LMTD_{i,CU} = [max(0, t_{iNOK+1}-TOUT_{CU})(tout_i-TIN_{CU}) \{max(0, t_{iNOK+1}-TOUT_{CU})+(tout_i-TIN_{CU})\}/2]^{1/3} + \delta
$$

$$
LMTD_{HU,j} = [max(0, TOUT_{HU}-t_{j1}) \; (TIN_{HU}-tout_j) \; \{max(0, TOUT_{HU}-t_{j1})+(TIN_{HU}-tout_j)\} \; /2]^{1/3} + \delta
$$

As discussed in Part I (Yee et al., 1990), δ is a small positive number, e.g. 10^{-6}, that is included in the approximation so that $LMTD$ cannot become zero and create numerical overflow problems.

The expressions in (8) involve nonsmooth terms since max operators are used. As discussed in Part I (Yee et al., 1990) these terms can be handled through the smooth approximation method by Duran and Grossmann (1986) and defined by the constraints of Kravanja and Grossmann (1989) (see equation (12) of Part I (Yee et al., 1990) of this series of papers).

The formulation (P1) for the simultaneous optimization or synthesis of the process and HEN involves the objective function in (7) subject to constraints (1) to (6) with variables x for flow rates, temperatures, and heat loads and variables w for the process parameters.

As mentioned previously, the heat integration portion of the combined process and HEN formulation can also be represented by an MINLP model. In this case, the formulation is similar to the one presented in Part II (Yee and Grossmann, 1990) of this series of papers. Constraints (1) to (6) are still applicable for this case. However, the nonsmooth terms in (8) can be eliminated by taking advantage of the binary variables *(z^, icu$_{i\%}$ zhujj* and defining additional constraints and variables to properly calculate the approach temperatures for selected exchangers *{dt^ dtcu$_{i\%}$ dihup.* Also, logical constraints are needed to assign values for the binary variables to declare the existence of matches between different pairs of streams. These constraints are as follows:

Logical constraints

The heat loads for each match are related to the 0*1 variables by the inequalities.

$$q_{ijk} - \text{H} \; z_{ijk} \; \pounds \; 0 \qquad i \in HP, \quad j \in CP, \quad k \in ST$$

$$qcu_i - \text{d} \; zcu_i \; \leq \; 0 \qquad ieHP \qquad\qquad (?)$$

$$qhu_j - 12 \; zhuj \; \leq \; 0 \qquad jeCP$$

$$z_{ijh} \quad {}^{2CU}i* \quad {}^{zku}j \; = \; \circ_* \; 1$$

where the corresponding upper bound *Cl* can be set to the smallest heat content of the two streams involved in the match.

Calculation of approach temperatures

In order to determine the temperature driving forces in the selected stream matches, the following inequalities apply,

$$dt_{ijk} \leq t_{i,k} - t_{j,k} + \Gamma\ (\ ^1 \sim\ ^2_{ijk}\ ) \qquad k \in ST, \quad i \in HP, \quad j \in CP$$

$$dt_{ijk+1} \leq t_{i,k+1} - t_{j,k+1} + r < 1 - hjk\ ) \qquad te^\wedge \qquad \in\!\ll\!P. \quad jeCP$$

$$dtcu_n \leq\ ^\wedge0^\wedge - rot/r^\wedge + r\ (\ 1\ -\ zcut\ ) \qquad /\in//\!\!»$$

$$dtcu_{i2} \leq touti - r/A^\wedge + r\ (\ 1\ -\ zcu_t\ ) \qquad ieHP \tag{10}$$

$$dthu_{j1} \leq TOUT_m - t_{jx,} + r\ (\ 1\ -\ ztoy\ ) \qquad jeCP$$

$$dthu_{j2} \leq JIN_{HU} - toutj + T\ (\ 1\ -\ zhuj\ ) \qquad jeCT$$

$$dt_{ijk}, \ dtcu_i, \ dthu_j \geq \varepsilon \qquad k \in ST, \quad i \in HP, \quad j \in CP$$

where r is an upper bound on the approach temperature and £ can be interpreted as the lowest allowable value for EMAT. Note that each of the approach temperature constraints only becomes active when its corresponding match is selected, i.e., z=L

With the use of binary variables, the objective function can explicitly acoount for fixed charges for the heat exchanger units. The objective function is defined by the following equation where *IMTD* is again approximated using the Chen equation (1987):

$$AON \quad F(wjc) + \sum_{ieHP} CCU\ qcu; \quad + \quad]\pounds \sum_{jeCP} CHU\ qhu_j \quad +$$

$$\sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} CF_{ij}\ z_{ijk} \quad + \quad \sum_{i \in HP} CF_{i,CU}\ zcu_i \quad +$$

$$\sum_{jeCP} CF_{HUj}\ zhu_j \quad + \tag{11}$$

$$\sum_{ieHP\ jeCP\ k \in ST} \quad /\ (U_{ij}\ [(dt_{ijk})\ (dt_{ijk+1})\ (dt_{ijk}+dt_{ijk+1})\ /2]^{1/3}\ )\ )\ ]^{\beta}_{ij} \quad +$$

$$\sum_{i \in HP} C_{i,CU}\ [\ qcu_i\ /\ (U_{i,CU}\ [dtcu_{i1}\ dtcu_{i2}\ \{dtcu_{i1}+dtcu_{i2}\}\ /2]^{1/3}\ )\ ]^{\beta}_{i,CU} \quad +$$

$$\sum_{jeCP} \quad Cmi;\ [\ qtu*;\ I\ QJuni\ ldthu_{;i}\ dthu_n\ \{dlhu_A+dlhu_n\}\ /2]^{l}\&\ )^{\beta}HVJ$$

The MINLP formulation (P2) for the simultaneous synthesis of process and HEN involves the objective function *6e\\ne6* in (11) subject to the constraints defined in equations (1) to (6) and (9) and (10) with flow, temperature, and heat load variables *x* and process parameters *w.*

REMARKS

Unlike the models presented in the two previous papers of this series, in both of the formulations, (P1) and (P2), presented above, the heat integration constraints in (2), (3) and (6) involve nonlinear terms. This is due to the fact that stream flow rates and inlet and outlet temperatures do not have fixed values. As a result, a higher computational requirement for the heat integration model can be expected, not only due to the additional constraints for the process model, but also due to the nonlinear constraints in the heat integration model. Furthermore, since these nonlinear terms involve bilinearities, the model is nonconvex in nature. Good starting points, therefore, may be necessary to ensure that the solution of the model is globally optimal. The initialization procedures proposed in Part I (Yee et al., 1990) for an NLP model and Part II (Yee and Grossmann, 1990) for an MINLP model can be readily applied following the selection of starting values for the process. Solution of the NLP model can be obtained by the use of any NLP solver such as MINOS (Murtagh and Saunders, 1985). For the solution of the MINLP models, the Combined Penalty Function/ Outer Approximation algorithm of Viswanathan and Grossmann (1989), which can handle nonconvex functions, has been applied resulting in very good solutions as will be shown in the example problems.

Also, in the above presentation, the formulation has been presented for the general case. Fewer constraints and variables may be required due to the specifics of a process model. For instance, in Example 1 in the next section which involves the heat integration of distillation streams, the condenser and reboiler stream temperatures can be assumed not undergoing a temperature change since the heat transfer is due to a phase change. As a result, the model is simplified due to the following:

- Fewer temperature variables are needed since all the stage temperatures for a condenser or reboiler stream are the same.
- « For exchanges between two constant temperature streams, only one stage can be used.
- Fewer terms are required for the heat balance constraints since they are based not on temperature change but on enthalpy change.
- Fewer terms are required to calculate the heat transfer driving force for the case of a reboiler stream exchanging heat with a condenser stream. In this case, the driving force is simply the difference of the two stream temperatures.

Other characteristics of the process may also lead to simplification of the model.

Finally, design constraints on the HEN, such as forbidden or restricted matches, can be easily incorporated into the formulations. For instance, in (P1) this simply accomplished by setting the heat

loads $q_{ijk}=0$ for a forbidden match; in (P2), this is accomplished by also setting the binary variable $z_{ijk}=0$. The formulations can also be slightly modified to account for the possibilities of hot-to-hot and cold-to-cold matches (see Yee and Grossmann, 1990). Finally, in formulation (P2), where binary variables are used to declare the existence of the heat exchangers, structural constraints, such as restrictions on stream splitting and the number of exchangers in the network can also be easily imposed.

In the next section, two examples are presented to illustrate the effectiveness of the proposed method.

EXAMPLE 1

A distillation sequencing problem is used to illustrate the significant savings which can be obtained through a simultaneous design approach for the process and HEN. The objective of the process is to separate a three-component mixture of A-B-C into the pure components with the problem data shown in Table 1. Separations are assumed to be sharp (100% recoveries) and the temperature difference between the reboiler and the condenser for each potential column is assumed to be constant (see Andrecovich and Westerberg, 1985, for a discussion on this assumption). Available utilities are cooling water and steam at three different pressures. In addition, the hot stream H1 and the cold stream C1 from elsewhere in the plant require heating and cooling, respectively, and thus are available for heat integration. The process superstructure for the distillation sequence is shown in Figure 4 where two distinct sequences are embedded. The selection of different columns involves different fixed and variable charges. The fixed charges for the columns are assumed to be temperature dependent. Heat exchangers are charged on a per unit area basis in addition to a fixed charge for each exchanger required.

For comparison, a design is first obtained through a sequential approach. Since no heat integration is considered in optimizing the process, only utilities are used for the required heating and cooling of the streams. Binary variables are used in the model to designate the existence of the columns and also to properly select the type of steam used in each reboiler. Annual cost based on charges for the columns and utilities are minimized. The MILP formulation for this problem is then as follows:

$$\min \quad X < i^* + P /,.) + <:\ll \pounds, \; q_i^{cond}$$

$$+ C_{lp} \sum_i q_i^{lp} + C_{mp} \sum_i q_i^{mp} + C_{hp} \sum_i q_i^{hp}$$

s.t. $/_1 + /_2 = 250$

$f_3 - 0.4 \, /_1 = 0$

$f_A - 09 \, /_2 = 0$

For columns $/ = 1, \; 2, \; 3, \; and \; 4,$

$$\frac{i_i^{cond} - 330}{330}] - U_\mu \; (1-y_i)$$

$f_i^{cond} \quad 2t\text{-}33O$ (12)

$f_i^{reb} - f_i^{cond} = \Delta T_i$

$420 - \pounds^* - \pounds^*MT \le U_t \; (l\text{-}z/)$

$460 - '^* - EMAT \le U_t \; (1\text{-}z^\wedge)$

$490 - \{? - EMAT \; Z \; U_t \; <l\text{-}z?)$

$q_i^{cond} = \gamma_i \, f_i$

ean4 $\cdot\,'\,\ll\,>$

$+ \; q_i^{hp} - q_i^{reb} = 0$

$q_i^{lp} - U_q \; z_i^{lp} \le 0$

$q_i^{mp} - U_q \; z_i^{mp} \le 0$

$q_i^{hp} - U_q \; z_i^{hp} \le 0$

$y_i \; 2/\backslash \; z_i^{lp} \% \; z^{\wedge \, tup} \; z^{\wedge \, hp} = 0, \; 1$

$\tilde{f}_i, \; \mu_i, \; q_i^{cond}, \; q_i^{reb}, \; q_i^{lp}, \; q_i^{mp}, \; q_i^{hp} \; \ll^\wedge \; ^\wedge$

In the above formulation, $/$ is the subscript for representing each of the four columns. The variables

I, I, and *q* represent flows to the column, temperatures of the condenser *(cond)* and rebofler *(reb)$_t$* and heat loads respectively. Binary variables *y* are used to designate the existence of each of the columns, while binary variables 2 are used to determine which steam, low pressure (*//?*), medium pressure *(mp)* or high pressure *(hp),* is used for a selected column */.* The choice of which steam to use also depends on a specified minimum approach temperature EMAT, which was set to be 5K in the optimization. The condenser and rebofler are assumed to be operated at a constant temperature difference of AT. The variable charge for each column (JI) is calculated based on the operating temperature of the condenser. Since ji is being minimized in the objective function, it will take on a nonzero value only when a particular column is selected where variable *y* for the column becomes one- Finally, parameters *U are* predetermined upper bounds.

The above MILP formulation which involves 16 binary variables (for the selection of columns as well as the type of steam used for the reboflers), 33 continuous variables and 44 constraints, can be solved to obtain the optimal process flowsheet shown in Figure 5. The optimal sequence utilizes columns 1 and 3 to first separate component A from the mixture followed by the separation of components B and C. For both columns, the condenser temperature is operated at 330K to minimize the respective variable charge)JL Also, hot utility cost is minimized by using *lp* steam for both reboflers.

With the process optimized, temperatures, flows and heat loads of the streams become fixed and a HEN can be synthesized to heat integrate the streams. Hot streams for the integration are the condenser streams along with stream H1, while cold streams are the reboiler streams along with stream C1. The method proposed in Part II of this series of paper (Yee and Grossmann, 1990) is used to generate the network. As mentioned previously, since the condenser and reboiler streams involve phase change, the heat balances for these streams are based on enthalpy change rather than on changes in stream temperature. Also, between streams with constant temperature, only one stage is required for the HEN representation. For streams H1 and C1, however, two stages are used to allow for series matching. With these modifications, the HEN model was solved and the combined separation sequence and HEN flowsheet is shown in Figure 6. Area and heat load requirements for each exchanger are shown in Table 2. The optimal design requires a total annual cost of $1,389,600/yr. Most of this cost is attributed to utilities requiring S838,300/yr, while the capital cost for the heat exchangers is $121,800/yr and for the columns is $429,500/yr.

In order to apply the proposed simultaneous approach, a combined superstructure is created by

embedding the HEN representation into the process superstructure. For the HEN representation, only one stage was used for matches between streams with constant temperature while two stages were used for matches involving streams H1 and C1 to allow for series matching. Binary variables are included in the overall model to designate the existence of matches as well as columns. The overall MINLP formulation corresponding to model (P2) required 172 constraints and 140 continuous and 54 binary variables. No specifications for HRAT or EMAT were given so that the optimization can select appropriate values to minimize cost The model was solved using the combined penalty function/ outer approximation approach of DICOPT++ by Viswanathan and Grossmann (1989) via MINOS (Murtagh and Saunders, 1985) and SCICONIC (SCICON, 1986). The solution was obtained in 3 major iterations using a total CPU time of 306 seconds on a VAX 6420. The optimal process and HEN flowsheet is shown in Figure 7 and the area and heat load requirements for the exchangers are shown in Table 3. The total annual cost required for this design is $971,800, which comprises of $282,900/yr for utilities, $255,90Q/yr for the HEN and $433,000/yr for the columns. This figure corresponds to a 30% reduction in cost compared to the sequential solution of Figure 6 which has an annual cost of $1,389,600/yr.

The main difference between the sequential and simultaneous solutions is the level of heat integration that can be accomplished. For both cases, the same separation sequence was selected. However, for the sequential case, the column temperatures were chosen to minimize the column capital cost without regard for the potential heat integration. As a result, the condenser temperature was set to 330K in order to minimize the variable charge ji for both columns. The disadvantage with this temperature selection is that cold stream C1 cannot be fully utiRzed to cool the condenser streams since its inlet temperature is 325K. In the simultaneous solution, however, the anticipation of the heat integration set the condenser temperatures at higher values (348K and 336K) to better utilize stream C1. Both condenser streams are matched with C1 to minimize the cooling water requirement In addition, since stream H1 is no longer required to heat up stream C1, it can match with both reboiier streams to minimize the steam requirement. The selected temperatures of the columns still only require the use of low pressure steam. It is also interesting to note that some of the temperature approaches are rather small (between 1 and 2K in exchangers 3,5 and 7).

Therefore, by the proper selection of the operating temperatures in the columns, the utility requirement for the process is drastically reduced. In fact, the simultaneous design requires a utility cost that is roughly two and a half times lower than the design by the sequential approach. Also, this design

requires seven heat exchangers instead of six. To achieve the higher level of heat integration, the simultaneous design requires about twice the area, but this additional area costs only $134,000/yr while reducing the utility requirement by over $550,000/yr. The increase in capital cost for the columns resulting from the higher condenser temperatures selected is also relatively insignificant compared to the utility savings.

Finally, it is interesting to analyze the design of Figure 7 in terms of a T-Q diagram (see Andrecovich and Westerberg, 1985). As can be seen from this diagram in Figure 8, the condenser and reboiler heat loads of 12×10^6 kJ/hr of column 1 (A/BC) can be fitted exactly between streams H1 and C1. For column 3 (B/C), the condenser and reboiler both have heat loads of 22.5×10^6 kJ/hr. Stream H1 supplies 18×10^6 kJ/hr of heat to the reboiler while stream C1 absorbs 10.9×10^6 kJ/hr of heat from the condenser. This particular heat load distribution allows a shift of temperatures that avoids having the temperature approaches becoming too small. In this way, column 3 requires 11.64×10^6 kJ/hr of cooling water and 4.5×10^6 kJ/hr of low pressure steam. The only other utility requirement is 7.14×10^6 kJ/hr of low pressure steam to supplement the heating of stream C1.

EXAMPLE 2

In this example, the simultaneous optimization of the process and its HEN is performed through an NLP model. The process flowsheet is obtained from an example previously investigated by Kravanja and Grossmann (1989). The problem data are given in Table 4, and the process flowsheet is shown in Figure 9. The objective of the process is to make product C from a feedstock containing reactants A and B and inert D. Feedstock F1 contains 60% A, 25% B, and 15% D and has a maximum flow rate of 10 kmol/sec. Prior to the reaction, the feedstock is compressed to a higher pressure by a single-stage compressor. The compressed stream is then mixed with a recycle stream and the combined stream is sent to the adiabatic reactor. The exothermic gas phase reaction is favorable for conditions of high pressure, low temperature, high concentration of reactant B and low concentration of inert D. The outlet stream from the reactor is sent to a flash unit where the lighter components, namely the reactants and inert, are separated from the heavier component C. The bottom stream P, which is the product stream, must contain at least 90% of component C. In addition, the flow of stream P must not exceed the maximum market demand of 1 kmol/s. The lighter components from the flash unit are recycled since the reactor conversion per pass is low. The recycled stream is compressed by a single-stage compressor and mixed with the compressed feedstock stream to form the reactant stream to the reactor. Also, a small portion of

the light ends from the flash unit is purged as a byproduct stream, P^, to avoid the buildup of the inert Both streams P and P^ must have a minimum temperature of 400 K.

The optimization of the flowsheet requires the determination of proper values for flows and temperatures for all the streams. For heat integration, the cold streams in the flowsheet to be heated involve the product and byproduct streams P and P^ and the feed stream to the reactor FR, while the hot stream to be cooled is the inlet stream of the flash unit FF. Since $max\{N_{ff}, N_c\}$ = 3, a three stage heat integration representation is set up and embedded into the process flowsheet The combined representation is shown in Figure 10.

Since the process flowsheet has a fixed structure, no binary variables are required. NLP Formulation (P1) is therefore used to account for the heat integration so that binary variables are not introduced into the combined process and heat integration model. The overall formulation contained 356 constraints and 343 variables, of which 76 constraints and 72 variables are for heat integration. Costs for the heat exchangers are based on the cost equations given by Kravanja and Glavic (1990) who use stream individual cost factors on a per unit area basis. Heat capacities for the streams are allowed to vary as a function of temperature. The model was solved using MINOS (Murtagh and Saunders, 1985) in 175 CPU seconds on a VAX 8800. The solution obtained is shown in Figure 11. For this solution, the total annual profit is maximized to $1,845,000. Note that the inlet and outlet temperatures of stream FR are the same and hence no match is required for this stream. Also, since the fixed charges for heat exchangers are not explicitly accounted for in the NLP model and no account is made for economy of scale in the cost equation, multiple exchangers are used for matches FF-P_{by} and FF-P. Therefore, a suboptimization on the HEN was performed to account for the fixed charges. Guthrie's correlations (Guthrie, 1969) for heat exchangers and boilers were used. The exchangers were merged without significant changes in costs. The final heat integrated design is shown in Figure 12 and the design specifications are shown in Table 5.

This solution compares very well with the ones presented in Kravanja and Grossmann (1989). First, they noted that for the sequential case where the flowsheet is optimized without regards for heat integration, a *toss* of $1,192,000 is actually incurred in the final design. Significant improvement is then made when heat integration is considered using the method of Duran and Grossmann (1986). However, the method can only consider the utility cost based on a given HRAT and does not consider the capital cost for the HEN. As a result, a *loss* of $292,000 is incurred in their final design for a value of

HRAT=30K. Rnally, Kravanja and Grossmann (1989) presented their solution which in turn is considerably better than the two previous solutions. Their model can account for the cost of area in the HEN and lead to a final design which yields an annual profit of $1,679,000. However, this solution is still roughly 10% lower than the profit obtained by the design derived by the proposed method. The primary reason for this difference is the fact that area considerations in the Kravanja and Grossmann model are based on strict vertical heat transfer. As a result, since the heat transfer coefficients of the streams in this example are quite different, the flexibility of allowing criss-cross heat transfer of the proposed method enabled a better design.

CONCLUSIONS

The potential for heat integration can be a very important factor when selecting the parameters for a process flowsheet An approach has been developed in this paper to simultaneously synthesize or optimize the process and its HEN. The approach involves incorporating the heat integration representation presented in Part I of this series of paper (Yee et al., 1990) with the process superstructure or flowsheet and optimizing the combined model. Unlike previous models for simultaneous optimization and heat integration, the proposed method does not require the specification of HRAT or EMAT, but rather optimizes them to minimize cost. The proposed approach also does not require the use of temperature intervals or any analysis based on the composite curves, such as determining the pinch location. Constraints for heat integration, such as forbidden, required, or restricted matches can be easily incorporated into the formulation. The method can also account for differences in heat transfer coefficients between the streams since no vertical matching is assumed. Last but not least, the method can actually generate the optimal HEN, defining the configuration, area requirement, number of units, and flows and temperatures.

In the combined model, heat integration is defined either by MINLP or NLP constraints. Both sets of constraints have been presented. The decision of whether or not to use binary variables can be based on the characteristics of the process model, i.e., *use* binary variables if the process model already requires them. The use of binaries provides a more accurate account of the HEN capital cost since fixed charges for requiring units can be charged explicitly. In addition, constraints on the network structure, such as the specification of no stream splits allowed, can be imposed easily with the use of binary variables. The expense, however, is that a larger computational time is required compared to the NLP case. The fact that some of the model constraints are nonconvex in nature means that more than one solution may exist

Therefore, good initialization of both the NLP and the MINLP problems may be needed to increase the likelihood for obtaining the global optimal solution.

The two examples presented have shown very clearly that the trade-offs between capital and utility costs can be properly modeled through the use of the proposed simultaneous approach. The comparison between the sequential and simultaneous solution in Example 1 has confirmed that heat integration must be anticipated at the stage of synthesizing or optimizing the process.

In this series of three papers, the heat integration representation introduced in Part I (Yee et al., 1990) has been applied to various problems with very encouraging results. Even though the heat integration problem is highly combinatorial, basic assumptions in the proposed models have lead to efficient solution times. The important aspect of the representation is that it does not follow the traditional route for solving heat integration problems- That is, it does not rely on the definition of temperature intervals, the specification of HRAT or EMAT, the location of the pinch point, or the analysis of the composite curves. Without this reliance on a heuristically-based procedure, the proposed models can explicitly and effectively account for the trade-offs between utility and capital costs. In fact, our results have indicated that heuristics may often fan when all types of costs are considered simultaneously.

ACKNOWLEDGEMENT

REFERENCES

1. Andrecovich, M.J. and Westerberg, A.W., "An MILP formulation for heat-integrated distillation sequence synthesis", *AIChE J.,* Vol. 31,1985, pp. 363.

2. Chen, J.J.J., "Letter to the Editors: Comments on Improvement on a Replacement for the Logarithmic Mean", *Chemical Engineering Science,* Vol. 42,1987, pp. 2488-2489.

3. Douglas, J.M., "A Hierarchical Decision Procedure for Process Synthesis", *AIChE* J., Vol. 31,1985, pp. 353-362.

4. Duran, MA and Grossmann, I.E., "Simultaneous Optimization and Heat Integration of Chemical Processes", *AIChE J.,* Vol. 32,1986, pp. 123-138.

5. Guthrie, K.M., "Capital Cost Estimating", *Chemical Engineering,* VoL 76,1969, pp. 114-142.

6. *IBM Mathematical Programming System Extended/370 (MPSX/3709), Basic Reference Manual,* White Plains, 1979.

7. Kravanja, Z. and Glavic, P., "Area Targeting for HEN through Simultaneous Optimization", *Manuscriptinpreparation,*1990.

8.   Kravanja, Z. and Grossmann, I.E., "PROSYN- An MINLP Process Synthesizer", *Presented at the Annual AIChE Meeting*, San Francisco, November 1989.

9.   Lang, Y.D., Biegler, L.T. and Grossmann, I.E., "Simultaneous Optimization and Heat Integration with Process Simulators", *Computers and Chemical Engineering*, Vol. 12, 1988, pp. 311-327.

10.   Linnhoff, B. and Townsend, D.W., "Designing Total Energy Systems by Systematic Methods", *I. Chem. E/SCI Conf.*, London, U.K., 1981.

11.   Murtagh, B.A. and Saunders, M.A., "MINOS 5.0 User's Guide", Tech. report SOL 83-20, Systems Optimization Laboratory, Dept. of Operations Research, Stanford University, 1985.

12.   Papoulias, S.A. and Grossmann, I.E., "A Structural Optimization Approach in Process Synthesis - III. Total Processing System", *Computers and Chemical Engineering*, Vol. 7, 1983, pp. 723-734.

13.   SCICON, *SCICONIC/VM User Guide*, SCICON Limited, London, 1986.

14.   Viswanathan, M. and Evans, L.B., "A Simultaneous Optimization and Heat Integration of Chemical Processes", *Presented at the Annual AIChE Meeting*, San Francisco, November 1989.

15.   Viswanathan, J. and Grossmann, I.E., "A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization", *Annual TIMS/ORSA - Canadian Operations Research Society*, Vancouver B.C., July 1989.

16.   Yee T.F., Grossmann, I.E., and Kravanja, Z., "Simultaneous Optimization Models for Heat Integration - I: Area and Energy Targeting and Modeling of Multi-stream Exchangers", *Submitted for publication*, 1990.

17.   Yee T.F. and Grossmann, I.E., "Simultaneous Optimization Models for Heat Integration - II: Heat Exchanger Network Synthesis", *Submitted for publication*, 1990.

STREAM DATA

Feed = 250 kgmol/hr

Mole fraction: A=0.6,   B=0.3,   C=0.1

	$T_{in}(K)$	$T_{out}(K)$	$\left(\dfrac{kJ}{hr\ K}\right)$
H1	450	375	400
C1	325	350	1200

Heat transfer coefficients = $1000\ \dfrac{kJ}{hr\,m^2 K}$ — & — for all matches

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AVAILABLE UTILITIES

Cooling Water (CW)	300-320 K	1.3 $(10^3\ \$\ hr/\ 10^6\ kJ\ yr)$
LP Steam (LP ST)	420 K	23
MP Steam (MP ST)	460 K	34
HP Steam (HP ST)	490 K	40

TEMPERATURE DIFFERENCE BETWEEN REBOILER AND CONDENSER

A/BC: 70 K

AB/C: 60 K

A/B: 43 K

B/C   3 8 K   minimum condenser temp. (Toond)=330 K

INVESTMENT DATA, HEAT DUTIES

	Base Fixed Charges (a) (ItfS/yr)	Variable Charges (p) $(10^3\ \$\ hr/kgmol\ yr)$	Heat Duty Coeff. fft $(10^6\ kJ/kgmol)$
A/BC:	32	0.27	0.048
AB/C:	55	1.15	0.095
A/B:	30	0.29	0.052
B/C	98	2.32	0.225

Investment cost for columns = a $[l+\pm sss\pounds z\pounds L]$ + ft [feed to column] $\dfrac{T}{330}$

Condenser duty = Reboiler duty = y[feed to column]

Annualized exchanger cost = 2000 + 35 [Area (m²)]

Table 1   Problem Data for Example 1

Exchanger	Area (nf)	Heat Load H000 kJ/hr)
1	659.17	12000
2	366.52	12000
3	160.24	12000
4	282.00	18000
5	1235.94	22500
6	432.69	22500

Table 2 Ex.1 Exchanger Area and Heat Loads for Sequential Solution

Exchanger	Area (nf)	Heat Load (1000 kJ/hr)
1	97.92	7142
2	1525.10	12000
3	1099.78	12000
4	473.67	11642
5	2117.20	10858
6	97.66	4500
7	1501.37	18000

Table 3 Ex.1 Exchanger Area and Heat Loads for Simultaneous Solution

STREAM DATA

	Composition	Cost - $/kmol	h (w/K-m^2)
Feed Fl	60% A	0.0245	
	25% B		
	15% D		
Product P	^90% C	0.2614	6200
Byproduct P$_{by}$		0.0163	64
Feed to Reactor FR			64
Feed to Flash Unit FF			64

$$Fl \leq 10 \text{ kmol/s}, \quad P \leq 1 \text{ kmol/s}$$

UTILITY DATA

	Cost	h (W/K-m^2)
Electricity	$0.03/(kW hr)	
Steam	$8.0/10^6 kJ	10000
Cooling Water	$0.7/10^6 kJ	6200

DESIGN SPECIFICATIONS

Reactor pressure, MPa	$2.5 \leq P_R \leq 15$
Inlet temperature (K)	$300 \leq T_{in} \leq 623$
Outlet temperature (K)	$365 \leq T_{out} \leq 623$

FLASH SEPARATION

Pressure, MPa	$0.15 \leq P \leq 15$
Temperature (K)	$300 \leq T \leq 500$

Operating time = 8500 hrs/yr

Table 4   Problem Data for Example 2

STREAM FLOWS

Feed F1	5.438	(kgmol/sec)
Product P	1	
Byproduct P_{by}	2.527	
Purge Rate (%)	15.7	

UTILITY REQUIREMENT

Electricity (MW)	2.883
Steam (10^9 MJ/yr)	0
Cooling Water (10^9 MJ/yr)	1.137

REACTOR DESIGN

Reactor pressure (MPa)	4.879
Inlet temperature (K)	367
Outlet temperature (K)	422
Conversion of B per pass (%)	27.0
Composition of inlet stream (%)	A: 54.4, B: 18.1, C: 1.2, D: 26.3

FLASH SEPARATOR DESIGN

Pressure (MPa)	4.391
Temperature (K)	333

EARNINGS (10^3 $/yr)

Product P	8000
Byproduct P_{by}	1264

EXPENSES (10^3 $/yr)

Feedstock F1	4078
HEN cost	900
Utility cost	1531
other	910

ANNUAL PROFIT (10^3 $/yr)

1845

Table 5   Results for Example 2

OPTIMIZED
PROCESS
DESIGN

cold streams

flow rates F_c
inlet temp. TIN_C
outlet temp. TOUTfc

hot streams

flow rates $^F H$
inlet temp. TIN_H
outlet temp.TOUT^

HEAT
EXCHANGER
NETWORK
DESIGN
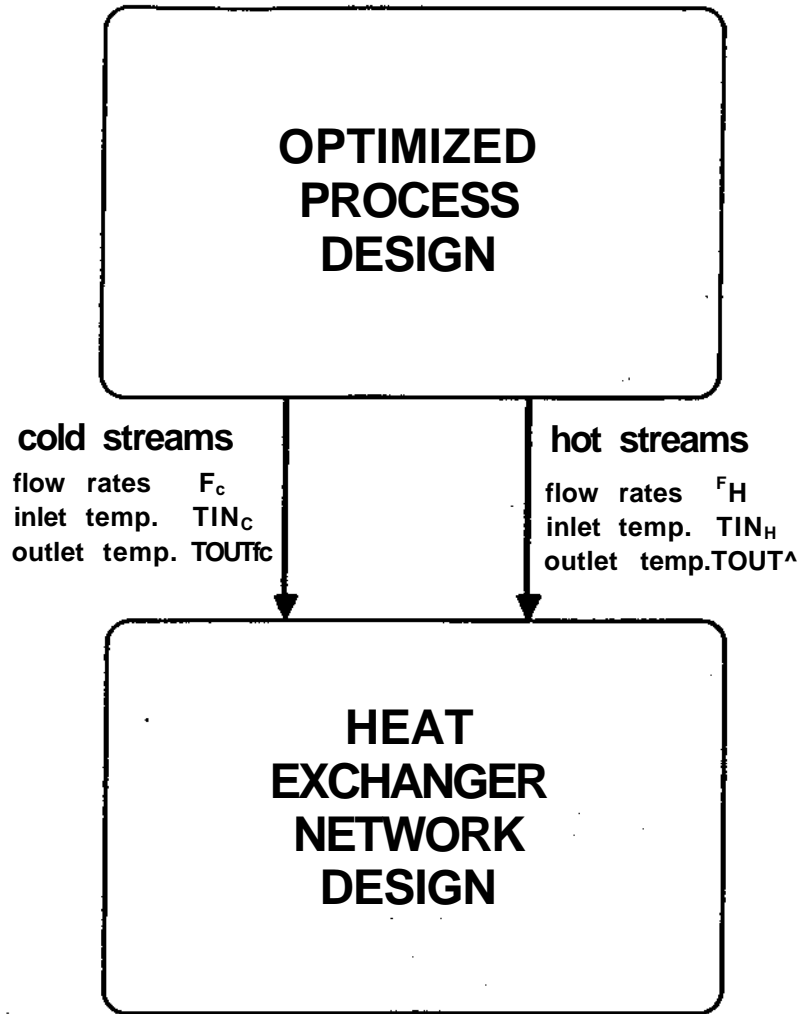
Rgure 1 Sequential Design for Process and Heat Exchanger Network
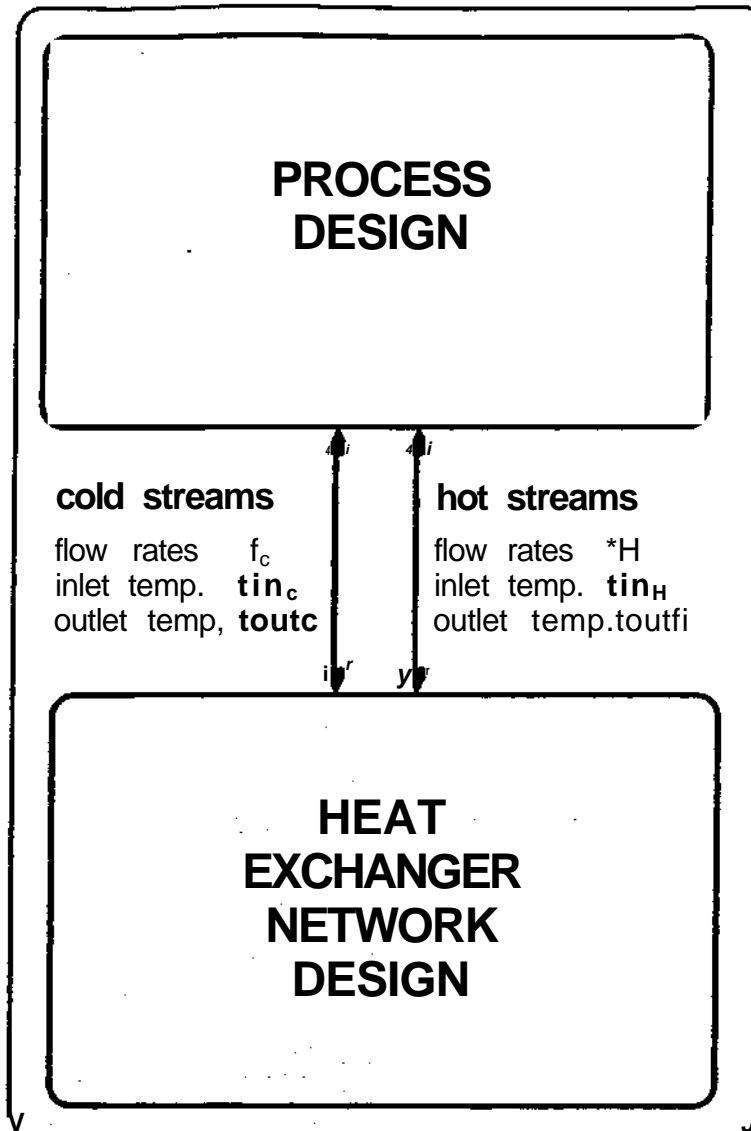
Rgure 2 Simultaneous Design for Process and Heat Exchanger Network
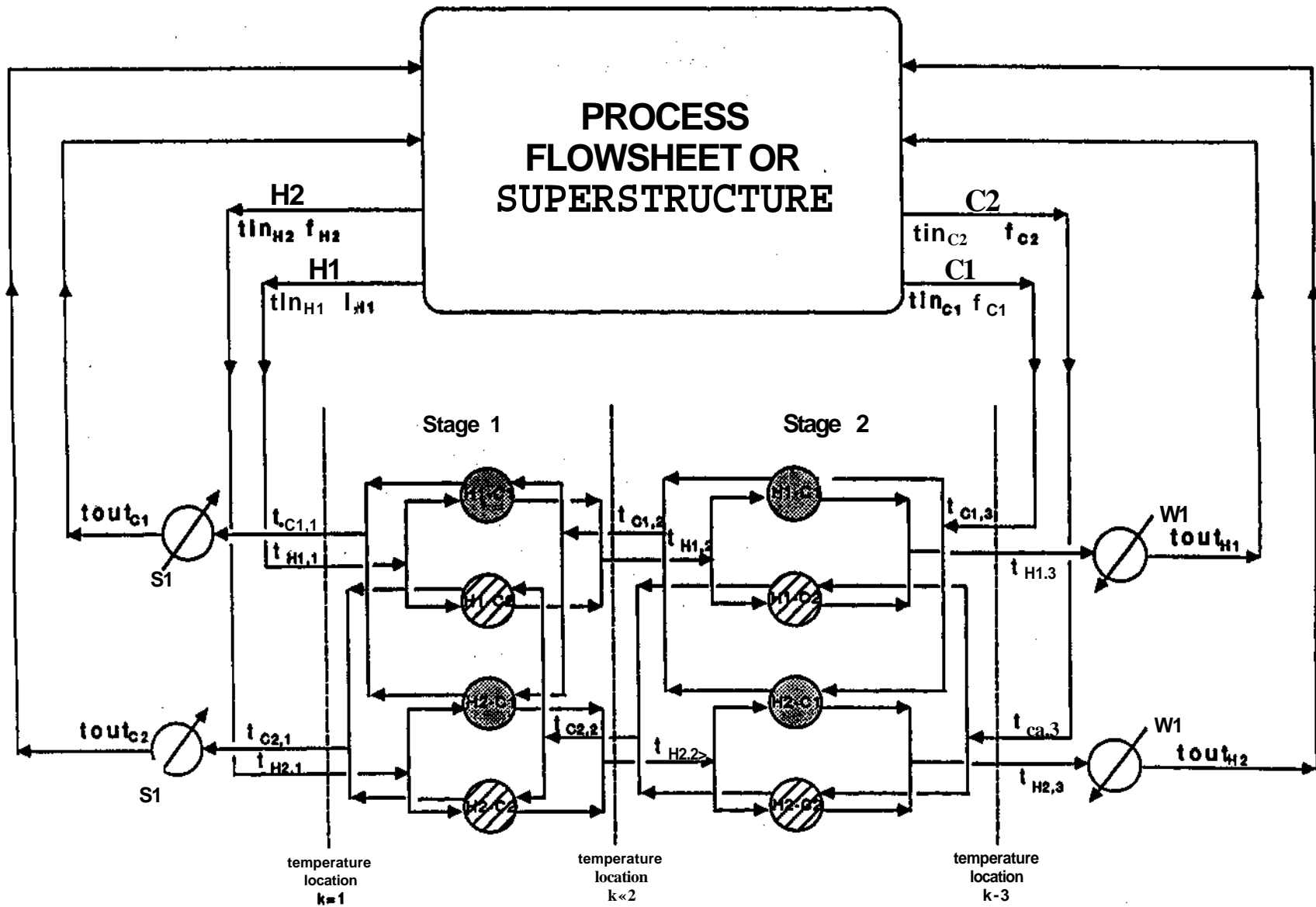
Figure 3   Combined Process and Heat Integration Representation
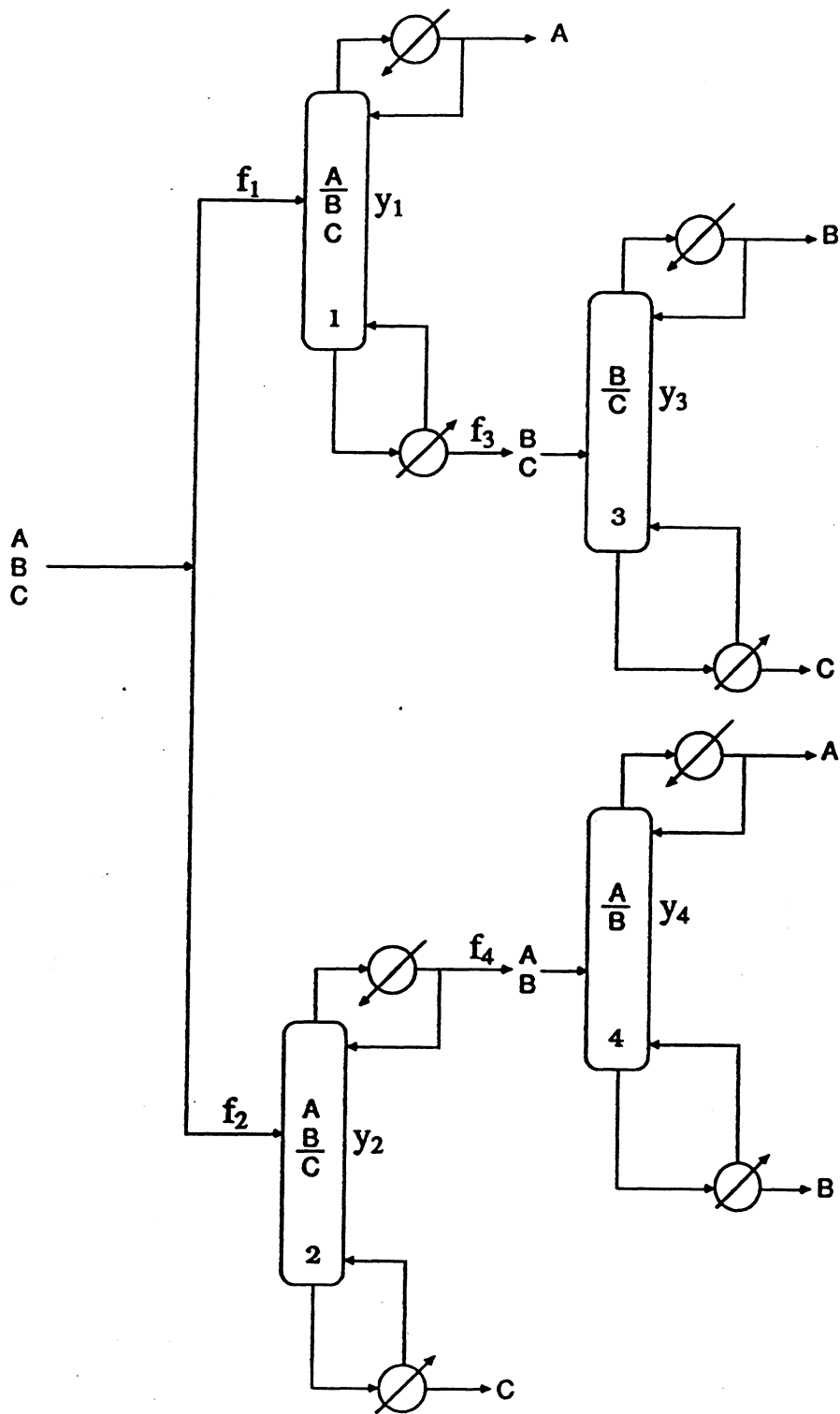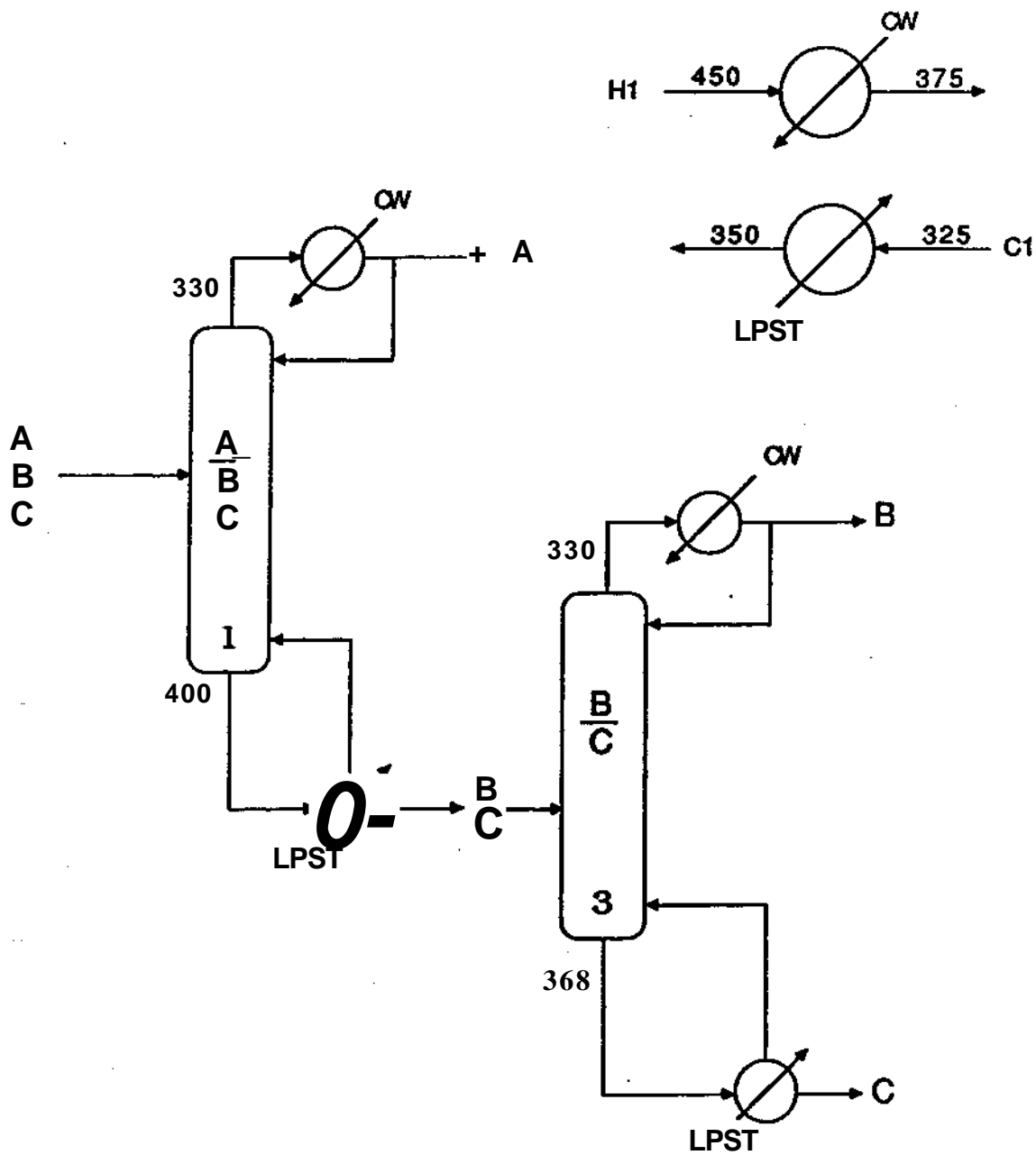
Figure 4   Process Superstructure for Example 1

Figure 5   Sequential Optimal Design for Distillation Sequence
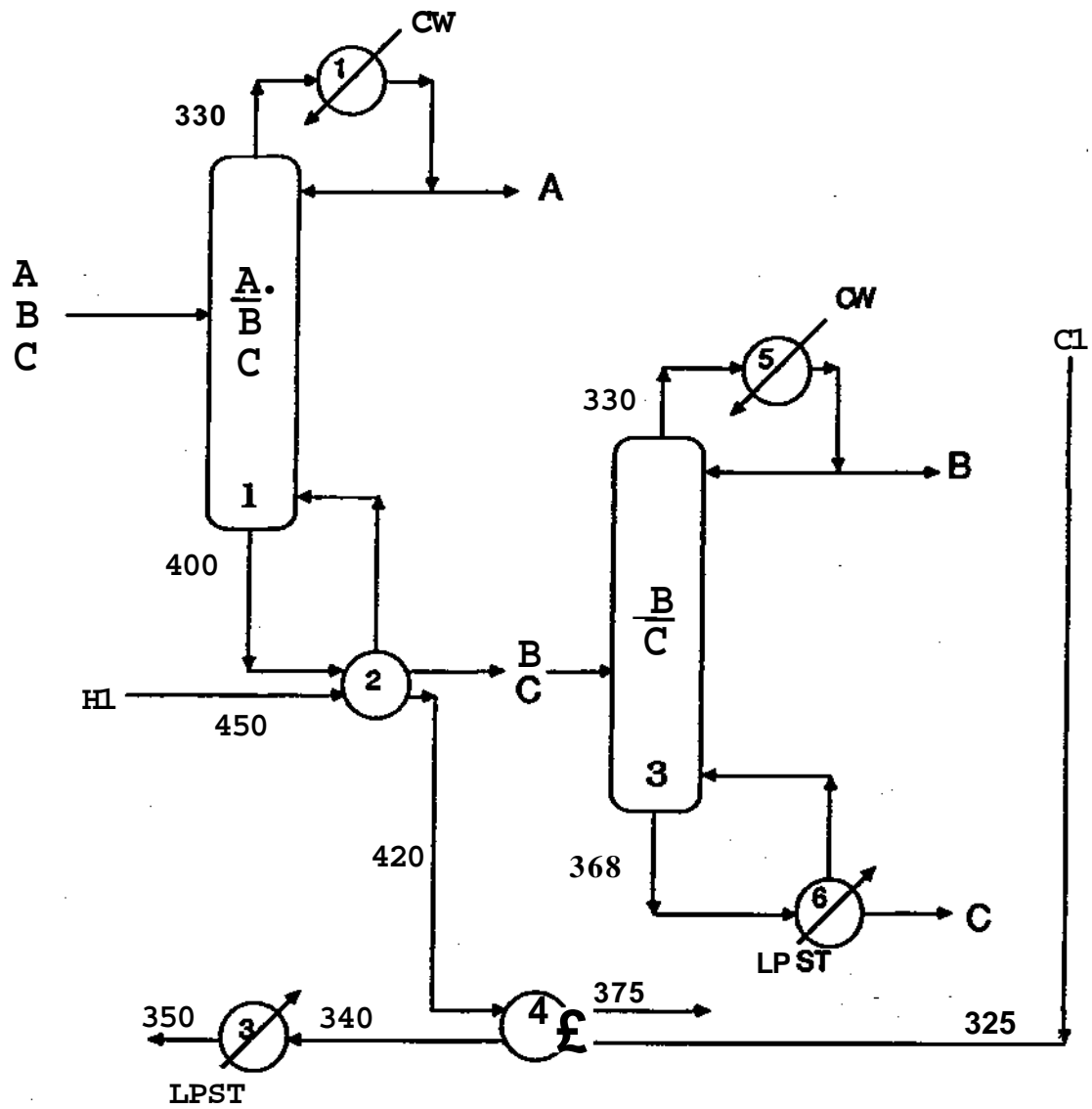
Figure 6 Optimal Process and HEN Design using Sequential Approach
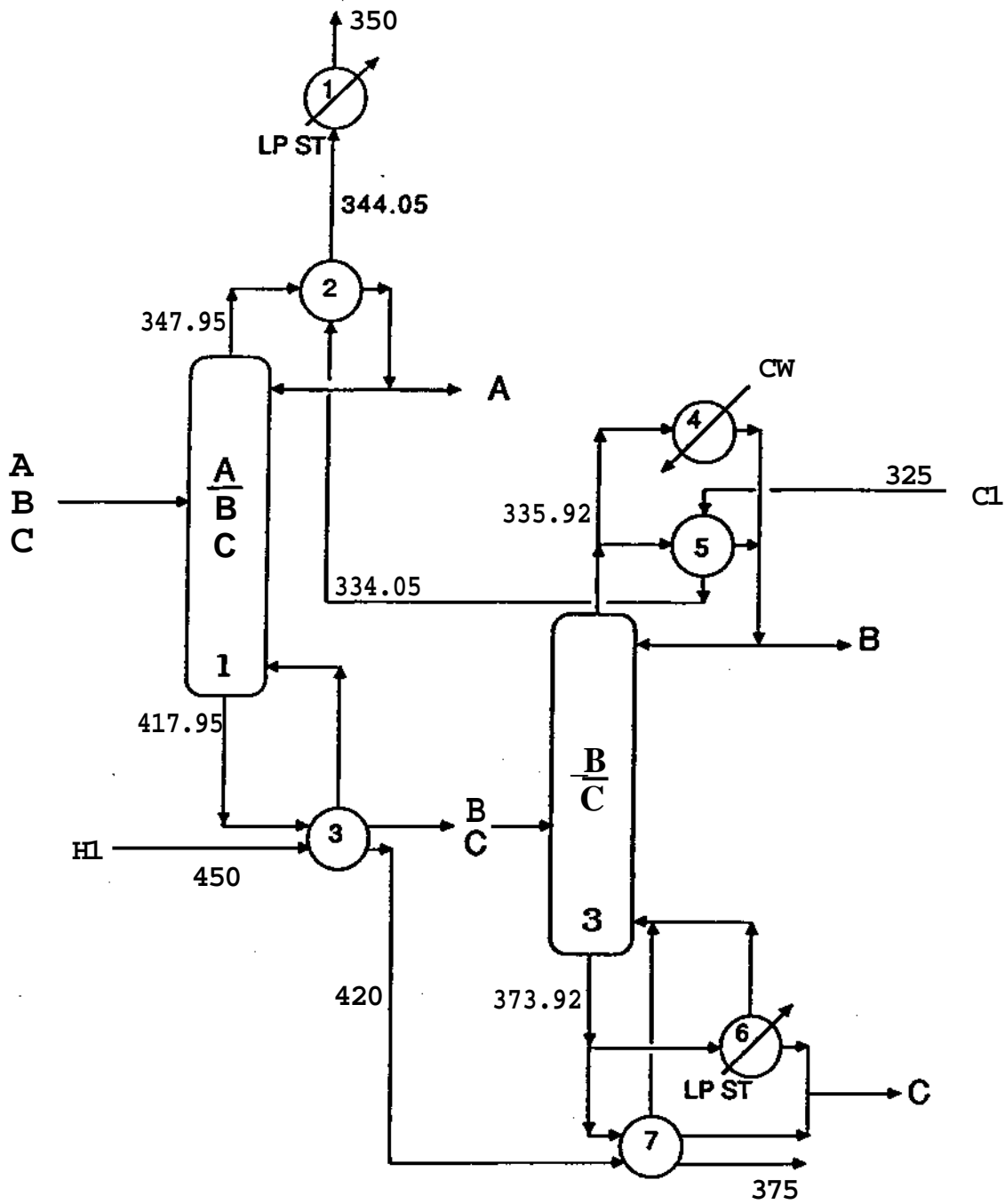
**Figure 7 Optimal Process and HEN Design using
Simultaneous Approach**
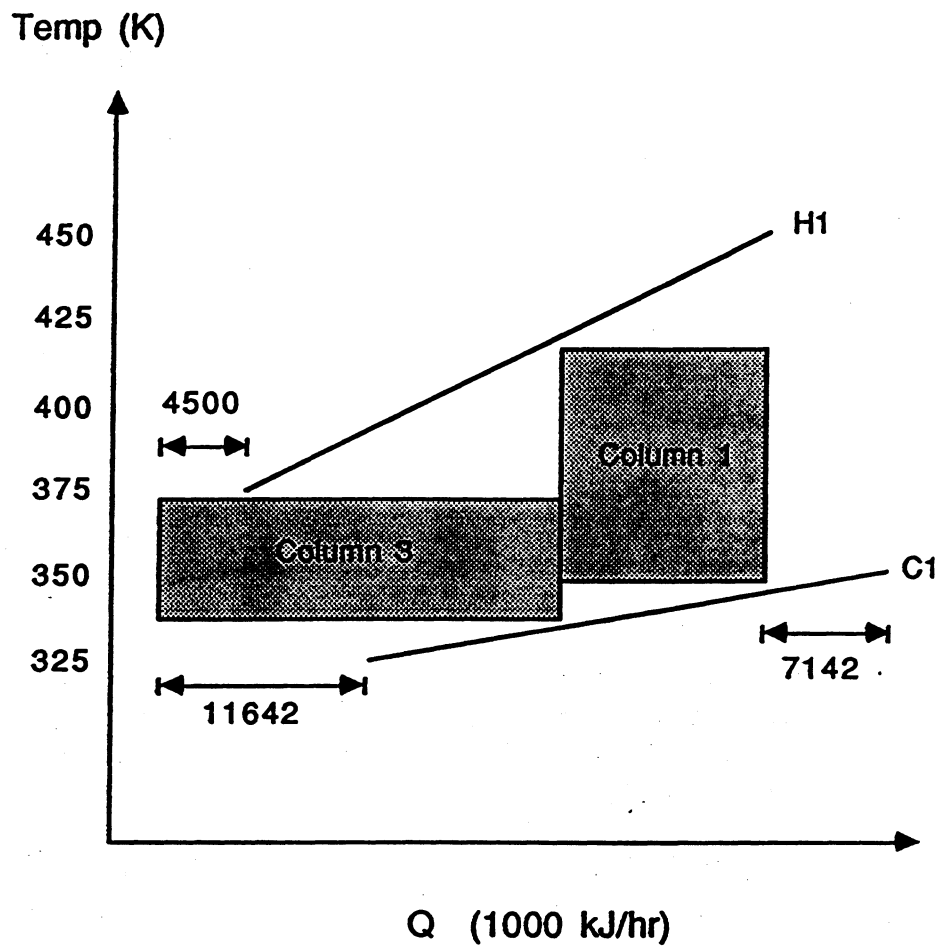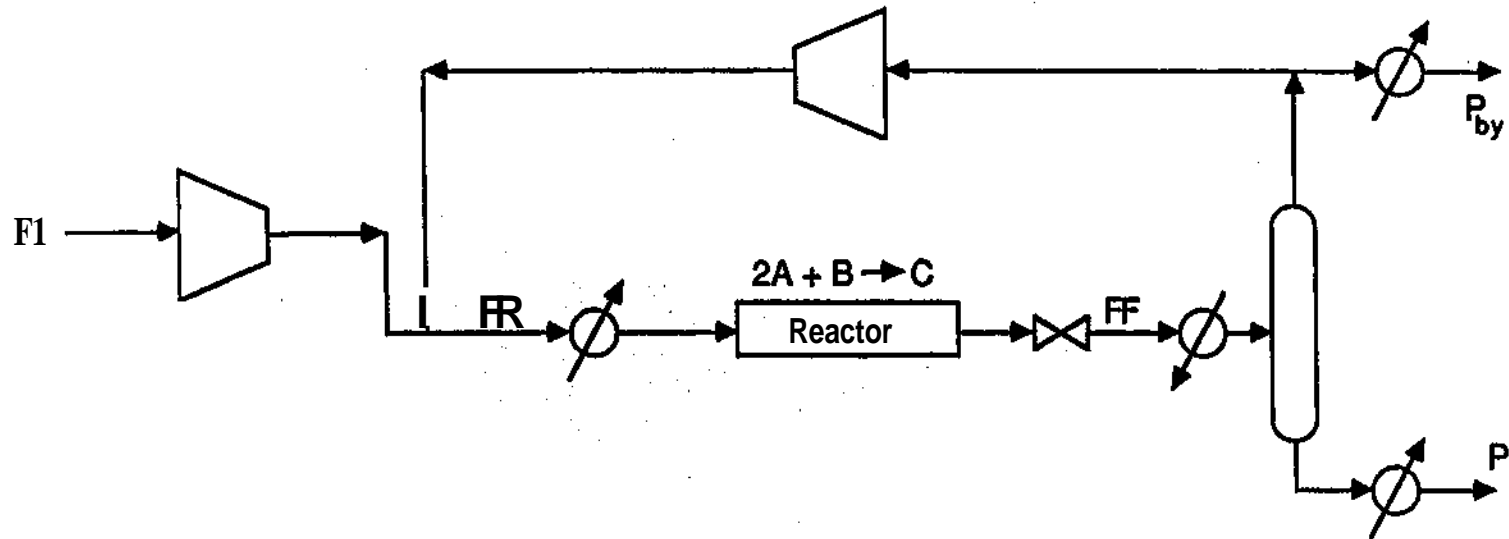
Figure 8 T-Q Diagram for Simultaneous Solution
of Example 1

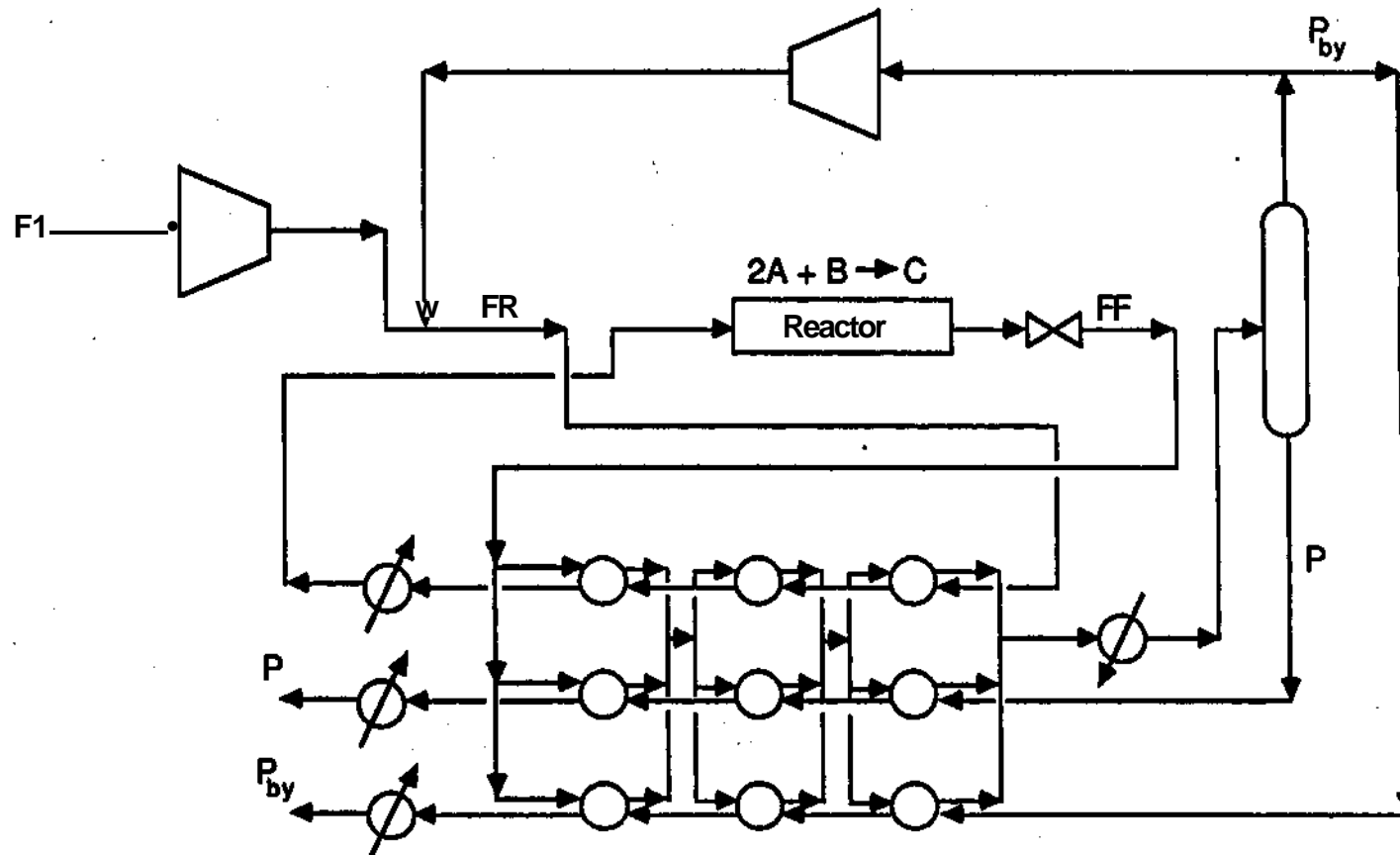**Figure 9   Process Flowsheet without Heat Integration
for Example 2**

Figure 10 Process Flowsheet with Embedded Heat Integration for Example 2
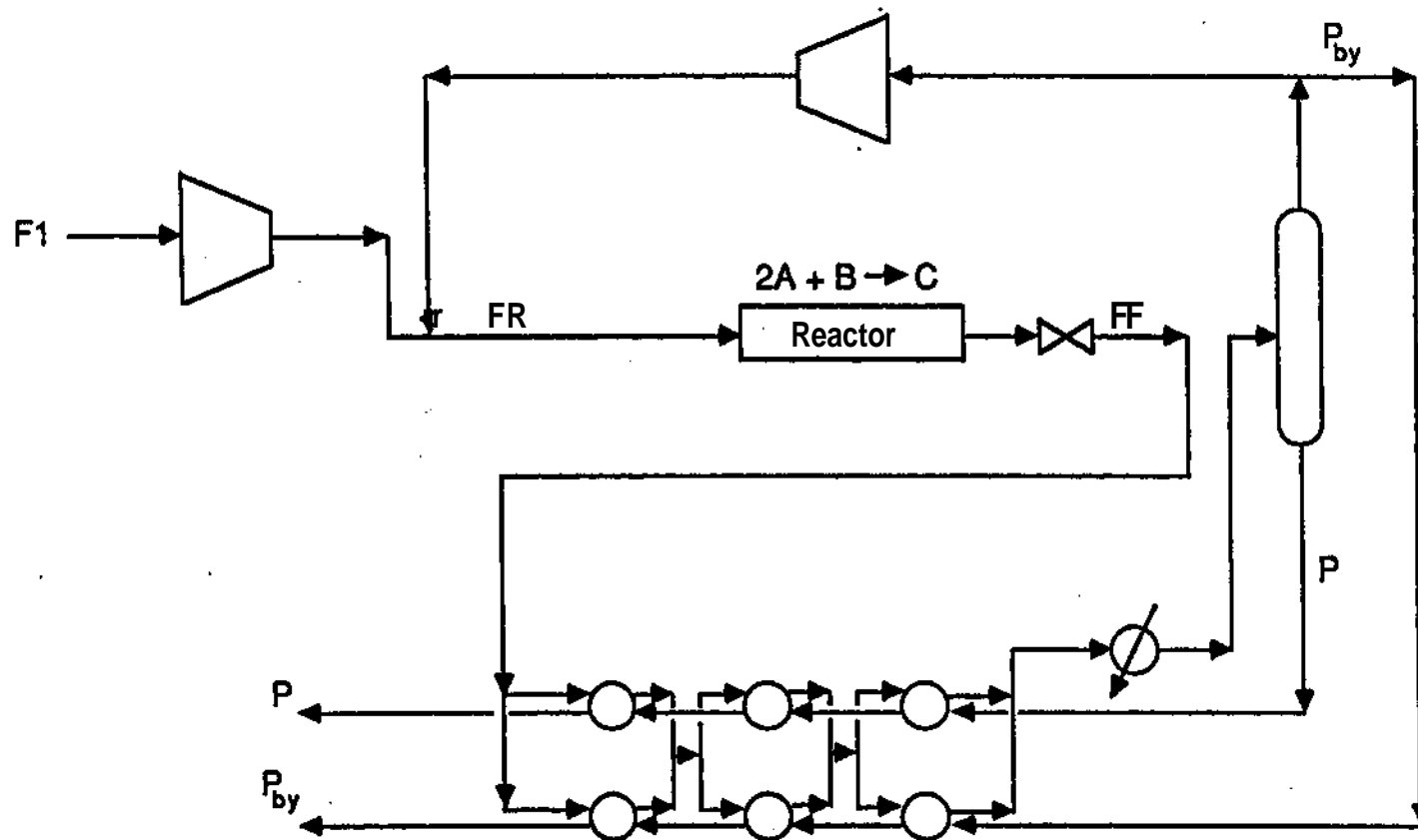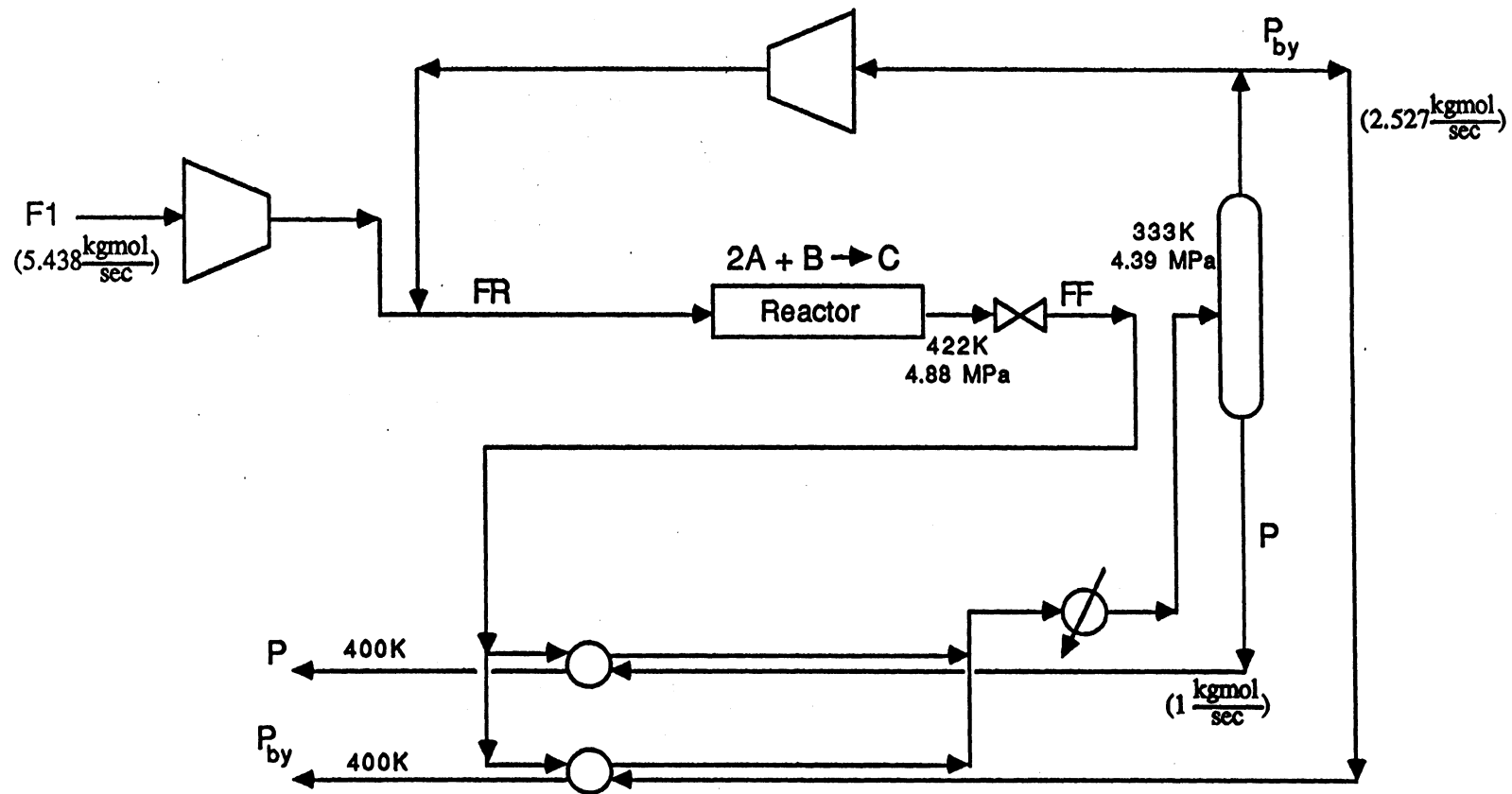
Figure 11   Optimal Process Flowsheet from Simultaneous Model Solution

Figure 12 Final Process Flowsheet for Example 2