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SIMULTANEOUS OPTIMIZATION MODELS FOR HEAT INTEGRATION—I. AREA AND ENERGY TARGETING AND MODELING OF MULTI-STREAM EXCHANGERS

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Abstract—In this paper, a simple yet general superstructure for heat integration is presented. The superstructure is a stage-wise representation where within each stage exchanges of heat can occur between each hot and cold stream. The proposed representation does not rely on any heuristics that are based on the concept of the pinch point, and its simplicity enables a *simultaneous* consideration for design factors without the limitations of a sequential analysis. In Part I of this three-part series of papers, an NLP model is first introduced for the exchanger networks. As will be shown, the model can *simultaneously* target for area and energy cost while properly accounting for the differences in heat transfer coefficients between the streams. Constraints on matches can also be easily handled. Furthermore, if a fixed utility consumption is specified, the model reduces to an area targeting model. In the last section of the paper, the proposed representation is also applied to the modeling of multi-stream exchangers. Examples for all the applications are presented to illustrate the efficiency and effectiveness of the proposed model.

INTRODUCTION

Over the past two decades, extensive research efforts have made considerable contributions to the heat integration problem. Gundersen and Naess (1988) provided an extensive review for heat exchanger network (HEN) design listing over 200 publications. In spite of the abundance of work in the area, most methods still have a number of limitations.

For instance, area targets typically rely on the assumption of strict vertical heat transfer [e.g. Townsend and Linnoff (1984) and Gundersen and Grossmann (1988)], and these methods often do not account for design constraints. A similar argument can be made for the number of units target for the network, where a simple heuristic equation determines the target. The question of whether one should partition the problem into subnetworks prior to determining the number of units target is another uncertainty. It is generally not simple to determine the proper heat recovery approach temperature (HRAT) at which utility targeting should be done.

In a typical HEN synthesis method (for a review see Part II—Yee and Grossmann, 1990) energy targeting for a fixed value of HRAT first establishes the utility requirement for the network. With utilities fixed, the number of units in the network is determined followed by an optimization of the exchanger area required. The limitation behind such a scheme, however, is that the effectiveness of each subsequent step relies heavily on the decisions of all the previous steps. Finally, in the heat integration problem that is performed simultaneously with the optimization of a flowsheet where the flows and temperatures of the streams are treated as variables, the main approach has been to enforce as a constraint the minimum utility target for fixed value of HRAT as in the method by Duran and Grossmann (1986). While this approach has the advantage of introducing a modest number of inequality constraints to the NLP or MINLP optimization, it does not consider the trade-off of area cost and utility cost. Furthermore, one cannot specify constraints on the stream matches in this approach.

While several methods have been proposed to address specific limitations in some of the problems cited above—these will be discussed later in the paper and in Parts II (Yee and Grossmann, 1990) and III (Yee *et al.*, 1990) of the series—these methods do not provide a unified representation where all the relevant design decisions can be optimized simultaneously with reasonable computational expense. This in fact is the objective of the heat integration models that will be presented in this series of papers. As will be shown, a simple stage-wise superstructure representation can be developed for the various heat integration problems. Based on this representation, optimization models that require very reasonable solution times are proposed to simultaneously account for the different design factors.

In this paper, the model is introduced and first presented for the *simultaneous* targeting of energy and area for heat exchanger networks with fixed flows and

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fixed supply are target temperatures. As will be shown, if a particular level of energy recovery is specified by fixing the utility requirement for the network, the model reduces to an area targeting formulation. Finally, it is shown that the proposed model can be incorporated in the optimization of a HEN involving multi-stream heat exchangers which can offer significant advantages over conventional single-hot-single-cold exchangers in certain applications, especially in cryogenic plants. In Part II (Yee and Grossmann, 1990), the model is formulated as a mixed integer nonlinear programming (MINLP) problem for the synthesis of heat exchanger networks. Annual cost, comprising of utility cost, area cost as well as fixed charges for exchanger units are optimized simultaneously. As will be shown, the model not only can account for design constraints such as forbidden, required or restricted matches, but also certain piping specifications (i.e. no stream splits). In Part III (Yee *et al.*, 1990) of the series, the formulation is extended to the simultaneous synthesis of process flowsheets and heat exchanger networks where the flows and temperatures are treated as variables. The important features of this model are that it optimizes both area and energy, and if desired, it provides the detailed network structures.

PROBLEM STATEMENT

In order to address the various heat integration problems in this series of three papers, it will be assumed that given are a set of hot process streams *HP* to be cooled and a set of cold process streams *CP* to be heated. Specified are also a set of hot utilities *HU* and a set of cold utilities *CU* and their corresponding temperatures. The various problems to be considered are as follows:

1. Area targeting—Given fixed flows, inlet and outlet temperatures and fixed utility requirement, determine minimum area cost, allowing for the possibility of nonvertical heat transfer and specification of constraints.
2. Simultaneous area and energy targeting—Given fixed flows, inlet and outlet temperatures, determine area and energy consumption to minimize cost allowing for nonvertical heat transfer and specification of constraints.
3. Modeling of multi-stream exchangers—Given fixed or variable flows, inlet and outlet temperatures, determine area requirement for a multi-stream exchanger allowing for specification of design constraints.
4. Synthesis—Given fixed flows, fixed or variable inlet and outlet temperatures, determine the energy consumption, number of exchangers, area requirement and network configuration which minimizes annual cost while allowing for specification of constraints on matches, heat loads and stream splitting.
5. Simultaneous process and HEN synthesis—Given the superstructure of a process with streams that can be heat integrated with variable flows, inlet and outlet temperatures, determine the optimal process and heat exchanger network design which minimize the annual cost while allowing for specification of design constraints.

Problems 1, 2 and 3 will be addressed in this paper, problem 4 in Part II (Yee and Grossmann, 1990) and problem 5 in Part III (Yee *et al.*, 1990). In these problems, the following assumptions will be made:

- Constant heat capacities
- Constant heat transfer coefficients
- Countercurrent heat exchangers

The next section will present a common superstructure representation that can be use to address all the problems cited above. In the proposed model, no heuristic assumptions are required, and all parameters need not be fixed but rather can be optimized. To simplify the problem, however, isothermal mixers will be assumed. As will be discussed later, this restriction simplifies the model significantly and allows for efficient and very reasonable solution times.

SUPERSTRUCTURE REPRESENTATION

The proposed representation for heat integration is a stage-wise superstructure which allows for different possiblities and sequences for matching streams. This superstructure can be viewed as an extension of the one presented in Grossmann and Sargent (1978) where within each stage potential exchanges between any pair of hot and cold streams can occur. It also resembles that of the spaghetti design concept brought forth by Linnhoff and coworkers, where the composite curves are divided into sections or a series of stages. In the spaghetti design, the number of stages is equal to the number of energy intervals (e.g. see Fig. 1). In each section of the composite curves, the corresponding cold streams are matched with the corresponding hot streams in order to obtain vertical heat transfer. As a result, spaghetti designs usually require a large number of exchangers.

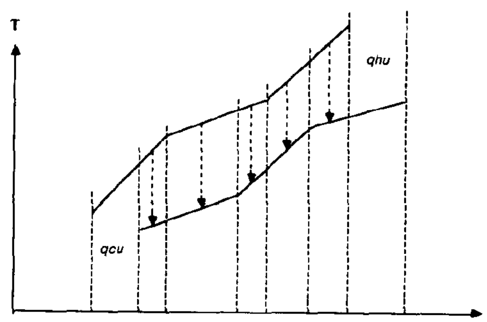

Fig. 1. Vertical heat transfer between composite curves leading to spaghetti design.

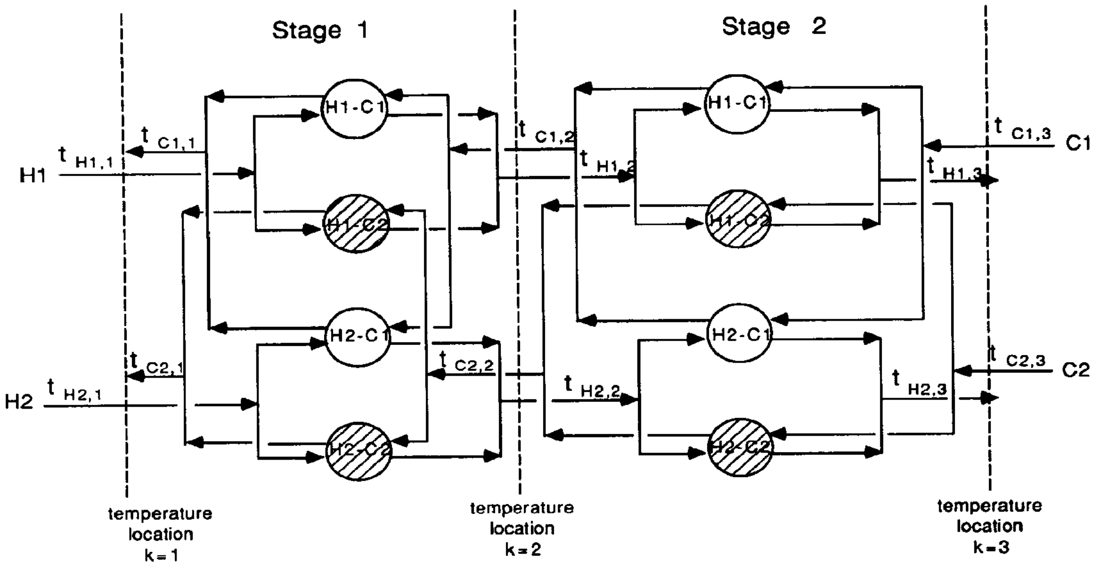

Fig. 2. Two-stage superstructure.

In the proposed superstructure, the number of stages does not have to be equal to the number of energy intervals since the temperatures corresponding to each stage will be treated as variables to be optimized. This in fact allows for opportunities for criss-cross heat exchange when streams have different heat transfer coefficients. In general, the number of stages required to model the heat integration will seldom be greater than either the number of hot streams N_H or the number of cold streams N_C. This is due to the fact that an optimal design usually does not require a large number of exchangers, meaning that a particular stream does not exchange heat with many streams.

The superstructure for the proposed model is then derived as follows (see Fig. 2):

1. Fix the number of stages, typically at $\max\{N_H, N_C\}$.
2. For each stage, the corresponding stream is split and directed to an exchanger for each potential match between each hot stream and each cold stream. The outlets of the exchangers are mixed which then defines the stream for the next stage.
3. The outlet temperatures of each stage are treated as variables.

Note that the derivation of the superstructure does not require the identification of the pinch point or the partitioning into subnetworks. An example of a superstructure involving two hot and two cold streams is shown in Fig. 2. The two stages are represented by eight exchangers, with four possible matches in each stage and variable temperatures between each stage. Note that alternative parallel and series configurations are embedded as well as possible rematching of streams. Also, for simplicity in the presentation, it will be assumed that the utilities are placed at the outlet of the superstructure.

Assuming isothermal mixing of the streams in the proposed superstructure can significantly simplify the model formulation. This restriction is illustrated in Fig. 3. The assumption specifies that the outlet temperature of a particular stream at each exchanger of a stage is the same as the outlet temperature of the stream in that stage. As shown in Fig. 3, for stream H1, the outlet temperatures of both exchanger H1–C1 and exchanger H1–C2 at each stage are assumed to be equal. The motivation behind this assumption is that by setting these temperatures to be the same, the nonlinear heat balance around each exchanger and the heat mixing equations can be eliminated. For each stream, only an overall heat balance must be performed within each stage. The simplification is especially relevant when the inlet heat capacity flowrates of the streams are fixed. For these cases, flow variables are no longer needed in the

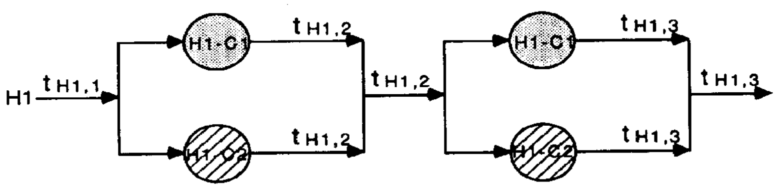

Fig. 3. Restrictions on split temperatures.

model. As a result, not only is the dimensionality of the problem reduced, but the feasible space of the problem can be defined by a set of *linear* constraints as will be shown later in the paper. The nonlinearities of the model, involving the calculation of areas using stage temperatures, are isolated in the objective function. The model therefore becomes very robust and can be solved with relative ease.

TARGETING MODEL

In this section an NLP formulation is proposed which *simultaneously* targets for energy and area for the minimum cost of a heat exchanger network. Similar to the recent NLP transshipment model of Colberg and Morari (1990), which is restricted to area targeting for a fixed heat recovery approach temperature (HRAT), the proposed model can account for differences in heat transfer coefficients as well as constraints on matches. In contrast, however, the model does not rely on any temperature interval definition nor any transshipment type constraints (Papoulias and Grossmann, 1983). Hence, the unique feature of the proposed method is that there is no need to fix HRAT, or the exchanger minimum approach temperature (EMAT), since these are treated as variables in the optimization. Furthermore, the solution of the model provides a feasible network with simple series and parallel configuration where required exchangers are the ones represented in the superstructure with nonzero heat loads. Finally, as will be shown, specification of the utility requirement in the model, which establishes the level of energy recovery, simplifies the formulation to an area targeting model.

In order to formulate the NLP model for area and energy targeting for the proposed superstructure described previously, the following definitions are necessary:

(i) Indices:

i = hot process or utility stream,
j = cold process or utility stream,
k = index for stage $1 \ldots NOK$ and temperature location $1 \ldots NOK + 1$;

(ii) Sets:

$HP = \{i \mid i$ is a hot process stream$\}$,
HU = hot utility,
$CP = \{j \mid j$ is a cold process stream$\}$,
CU = cold utility,
$ST = \{k \mid k$ is a stage in the superstructure, $k = 1, \ldots NOK\}$;

(iii) Parameters:

TIN = inlet temperature of stream,
$TOUT$ = outlet temperature of stream,
F = heat capacity flow rate,
U = overall heat transfer coefficient,
CCU = per unit cost for cold utility,
CHU = per unit cost for hot utility,
CF = fixed charge for exchangers,
C = area cost coefficient,
B = exponent for area cost,
NOK = total number of stages.
QCU = total cold utility usage,
QHU = total hot utility usage;

(iv) Variables:

q_{ijk} = heat exchanged between hot process stream i and cold process stream j in stage k,
qcu_i = heat exchanged between hot stream i and cold utility,
qhu_j = heat exchanged between hot utility and cold stream j,
$t_{i,k}$ = temperature of hot stream i at hot end of stage k,
$t_{j,k}$ = temperature of cold stream j at hot end of stage k.

With the definitions above, the formulation can now be presented. In the superstructure, utility streams can in general be treated as process streams with unknown flowrates. However, for simplicity in the presentation, utility streams are matched only at the outlet of the superstructure while assuming that only one type of hot and one type of cold utilities are available. These assumptions, of course, can easily be relaxed.

Overall heat balance for each stream

An overall heat balance is needed to ensure sufficient heating or cooling of each process stream. The constraints specify that the overall heat transfer requirement of each stream must equal the sum of the heat it exchanges with other process streams at each stage plus the exchange with the utility stream:

$$(TIN_i - TOUT_i)F_i = \sum_{k \in ST} \sum_{j \in CP} q_{ijk} + qcu_i, \quad i \in HP,$$

$$(TOUT_j - TIN_j)F_j = \sum_{k \in ST} \sum_{i \in HP} q_{ijk} + qhu_j, \quad j \in CP. \tag{1}$$

Heat balance at each stage

An energy balance is also needed at each stage of the superstructure to determine the temperatures. Note that for a superstructure with NOK stages, $NOK + 1$ temperatures are involved. This takes into consideration the fact that for two adjacent stages, the outlet temperature of this first stage corresponds to the inlet temperature of the second stage. To properly define the temperature variables and stages, the index k is used. The set $k = 1 \ldots NOK$ is used to represent the NOK stages of the superstructure, while the set $k = 1 \ldots NOK + 1$ is used to define the temperature location in the superstructure (see Fig. 2). In both cases, stage or temperature location

$k = 1$ involves the highest temperatures. The heat balances for each stage are thus as follows:

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

$$(t_{j,k} - t_{j,k+1})F_j = \sum_{i \in HP} q_{ijk} \quad k \in ST, \quad j \in CP. \quad (2)$$

Assignment of superstructure inlet temperatures

Fixed inlet temperatures of the process streams (TIN) are assumed and assigned as the inlet temperatures to the superstructure. For hot streams, the superstructure inlet corresponds to temperature location $k = 1$, while for cold streams, the inlet corresponds to location $k = NOK + 1$:

$$TIN_i = t_{i,1}, \quad i \in HP,$$

$$TIN_j = t_{j,NOK+1}, \quad j \in CP. \quad (3)$$

Feasibility of temperatures

Constraints are also needed to specify a monotonic decrease of temperature at each successive stage k. In addition, a bound is set for the outlet temperature of each stream superstructure at the respective stream's outlet temperature. Note that the outlet temperature of each stream at its last stage does not necessarily correspond to the stream's target temperature since utility exchanges can occur at the outlet of the superstructure:

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

$$t_{j,k} \geqslant t_{j,k+1}, \quad k \in ST, \quad j \in CP,$$

$$TOUT_i \leqslant t_{i,NOK+1}, \quad i \in HP,$$

$$TOUT_j \geqslant t_{j,1}, \quad j \in CP. \quad (4)$$

Hot and cold utility load

Hot (qhu_j) and cold (qcu_i) utility requirements are determined for each process stream in terms of the outlet temperature in the last stage and the target temperature for that stream. The following constraints are for the utility heat load requirements:

$$(t_{i,NOK+1} - TOUT_i)F_i = qcu_i, \quad i \in HP,$$

$$(TOUT_j - t_{j,1})F_j = qhu_j, \quad j \in CP. \quad (5)$$

Constraints (1–5) above comprise the linear equations and inequalities that are needed to define the feasible region for the targeting models.

Objective function

In the formulation, the targeted quantities can be placed explicitly in the objective function. Utility requirements for the network can be expressed as the sum of the utility required by each process stream:

$$\sum_{i \in HP} qcu_i \quad \text{cold utilities},$$

$$\sum_{j \in CP} qhu_j, \quad \text{hot utilities}. \quad (6)$$

Area requirement, however, requires a nonlinear calculation by the following terms:

$$\sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} [q_{ijk}/(U_{ij} LMTD_{ijk})]. \quad (7)$$

In general, an approximation for the $LMTD$ term is in order to avoid numerical difficulties when the approach temperatures of both sides of the exchanger are equal. In this paper, the Chen approximation (1987) is used:

$$LMTD_{ijk} \approx \left[(dt_{ijk})(dt_{ijk+1}) \frac{dt_{ijk} + dt_{ijk+1}}{2} \right]^{1/3}, \quad (8)$$

where dt_{ijk} and dt_{ijk+1} represent the approach temperatures for exchanger (i, j) in stage k.

Other well known approximations are:

(a) Paterson(1984):

$$LMTD \approx \frac{2}{3}\sqrt{dt_{ijk}\, dt_{ijk+1}} + \frac{1}{3}\frac{dt_{ijk} + dt_{ijk+1}}{2}; \quad (9a)$$

(b) Chen (1987) extending Underwood (1970):

$$LMTD^{0.3275} \approx \tfrac{1}{2}(dt_{ijk}^{0.3275} + dt_{ijk+1}^{0.3275}). \quad (9b)$$

As compared to the approximations of equations (9), the Chen approximation has the important advantage that when either dt_{ijk} or dt_{ijk+1} equals zero, the driving force will be approximated to be zero. For the other two approximations, however, a nonzero value may still be predicted when either dt_{ijk} or dt_{ijk+1} equals zero. Therefore, to avoid this inaccuracy, the Chen approximation in equation (8) is used in the proposed formulation. It should be noted, however, that whereas the Paterson approximation tends to slightly overestimate the driving force (thus underestimating the area requirement), the Chen approximation of equation (8) tends to slightly underestimate the driving force (thus overestimating the area requirement).

Also, in order to determine the driving forces, the approach temperatures, dt_{ijk} and dt_{ijk+1} need to be calculated for every match (i, j) in stage k. Due to the simplifying assumption for isothermal mixing, stage temperatures can be used for the calculation. It should be noted that nonnegative approach temperatures are only required for exchangers with positive heat loads. For exchangers not transferring heat, the stage temperatures should be free to assume any value since the corresponding heat loads are zero. In order to handle the case when an approach temperature of an exchanger with zero heat load involves a cold stream stage temperature t_{jk} that is larger than the hot stream stage temperature t_{ik}, the following equation can be used:

$$dt_{ijk} = \max\{0, t_{ik} - t_{jk}\}. \quad (10)$$

Note that when t_{jk} is larger than t_{ik}, the approach temperature is set to zero. There is no need to explicitly define the variables dt_{ijk} in the model as these can be substituted into equation (8) which in turn is substituted in the objective function term in (7). To ensure the area expression of equation (7) remains numerically stable, a very small positive tolerance δ, e.g. 10^{-6}, is added to the denominator to prevent division by zero.

The use of max operators in (10), however, introduces nonsmooth terms into the objective function. To overcome the nondifferentiability of these terms, the smooth approximation by Duran and Grossmann (1986) is used;

$$dt_{ijk} = \max\{0, t_{ik} - t_{jk}\} = \begin{cases} t_{ik} - t_{jk} & \text{if } t_{ik} - t_{jk} \geq \epsilon, \\ [\epsilon/\exp(1)]\exp[(t_{ik} - t_{jk})/\epsilon] & \text{otherwise,} \end{cases} \quad (11)$$

where ϵ is a small positive number. This approximation basically ensures continuity for both the function and its derivative at ϵ yet maintaining relatively small approximation errors if ϵ is selected to be sufficiently small (e.g. $10^{-8} \leq \epsilon \leq 10^{-4}$).

The Duran and Grossmann approximation can be easily incorporated into an NLP solver such as MINOS (Murtagh and Saunders, 1985) through an equation modeling system such as GAMS (Brooke *et al.*, 1988) by the following equation by Kravanja and Grossmann (1989):

$$dt_{ijk} = \max[0, t_{ik} - t_{jk}] \approx \max\langle \min\{\epsilon, [\epsilon/\exp(1)] \times \exp[\min(40, (t_{ik} - t_{jk})/\epsilon)]\}, t_{ik} - t_{jk} \rangle. \quad (12)$$

Here, the term $\min\{40, (t_{ik} - t_{jk})/\epsilon\}$ is specified simply to avoid any numerical overflow when $(t_{ik} - t_{jk})/\epsilon$ is large. These terms in (12) are directly substituted in the objective function to calculate the area required.

For the simultaneous optimization of energy and area targets, the objective function involves cost terms for both utilities and area. When the utility requirement is fixed in the formulation, the simultaneous model reduces to a model which determines the area target for the particular level of energy recovery. With the definitions and discussions above, the NLP formulations for the two targeting cases are as follows:

(a) NLP1—simultaneous energy and area targeting formulation

$$\min CCU \sum_{i \in HP} qcu_i + CHU \sum_{j \in CP} qhu_j + C_{ij} \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} [q_{ijk}/(U_{ij} LMTD_{ijk})]B_{ij} + C_{i,\mathrm{CU}} \sum_{i \in HP} [qcu_i/(U_{i,\mathrm{CU}} LMTD_{i,\mathrm{CU}})]B_{i,\mathrm{CU}} + C_{\mathrm{HU},j} \sum_{j \in CP} [qhu_j/(U_{\mathrm{HU},j} LMTD_{\mathrm{HU},j})]B_{\mathrm{HU},j},$$

$$\text{s.t. constraints (1–5)}, \ t, q \geq 0, \quad \text{(NLP1)}$$

and where equation (12) is substituted for the max expressions for the temperature approaches in the *LMTD* terms [see equation (8)]:

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

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

$$LMTD_{\mathrm{HU},j} = [\max(0, TOUT_{\mathrm{HU}} - t_{j1}) \times (TIN_{\mathrm{HU}} - TOUT_j) \times \{\max(0, TOUT_{\mathrm{HU}} - t_{j1}) + (TIN_{\mathrm{HU}} - TOUT_j)\}/2]^{1/3} + \delta. \quad (13)$$

In this formulation for simultaneous energy and area targeting, the objective function accounts for the trade-off between annual energy and area cost. The utility cost is charged on a per unit of heat load basis, while the area can be charged on a cost per unit basis or by an equation with fractional exponent, B to reflect the economy of scale.

It should be noted that in (NLP1) heat loads with infeasible temperature approaches will be set to zero provided that sufficiently small values for ϵ and δ are selected in (11) and (13). This follows from the fact that in this case the denominator of the investment cost terms in (NLP1) will take on very small values which greatly increases the cost of heat exchange. In our experience, the choices of $\epsilon = 10^{-4}$ and $\delta = 10^{-6}$ have shown to be satisfactory to accomplish this objective without producing serious ill-conditioning of the objective function.

(b) NLP—area targeting formulation

The simultaneous energy and area targeting formulation (NLP1) can be modified for area targeting simply by fixing the utility requirement for network and changing the objective function to minimize the total area requirement. The formulation is as follows:

$$\min \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} [q_{ijk}/(U_{ij} LMTD_{ijk})] + \sum_{i \in HP} [qcu_i/(U_{i,\mathrm{CU}} LMTD_{i,\mathrm{CU}})] + \sum_{j \in CP} [qhu_j/(U_{\mathrm{HU},j} LMTD_{\mathrm{HU},j})],$$

$$\text{s.t. constraints (1–5)}, \quad \text{(NLP2)}$$

$$\sum_{i \in HP} qcu_i = QCU,$$

$$\sum_{j \in CP} qhu_j = QHU, \quad t, q \geq 0.$$

In formulation (NLP2), QCU and QHU represent the fixed amount of cooling and heating utility requirement for the network, respectively. Solution of the formulation, therefore, determines the area target for a network with the specified hot and cold utility requirement.

It should be noted that in both (NLP1) and (NLP2), constraints on matches can be easily incorporated into the formulations. Forbidden matches can be specified by fixing the relevant heat load variables to zero. Restricted and required matches can be declared through the constraints which sum up the relevant heat loads for the match through all stages, and are bounded above by the restricted heat load value or else bounded below by the required heat load value. Finally, the solution to this problem will generate a heat exchanger network configuration. For the case when only the area is minimized in (NLP2), or a linear cost of area is used in (NLP1), the configuration will usually exhibit a rather large number of units. For problem (NLP1), if a cost exponent is used for the areas, the number of units will generally decrease. The synthesis of the network structure, however, will be addressed in Part II (Yee and Grossmann, 1990).

REMARKS

The attractive feature of both proposed models, (NLP1) and (NLP2), is that constraints (1–5) which define the feasible space, are linear. This has the effect that when applying a reduced gradient method (e.g. MINOS, Murtagh and Saunders, 1985) to the NLP, superlinear convergence can be guaranteed. As a result, the problem can be solved efficiently with reasonable computational time. It should be noted, however, that the nonlinearities in the objective function (7) may lead to more than one local optimal solution due to their nonconvex nature. But, unlike other heat exchanger network models, the nonconvex terms appear only in the objective function (Floudas *et al.*, 1986; Yee and Grossmann, 1988; Floudas and Ciric, 1989). To increase the likelihood of obtaining the global optimal solution, an initialization procedure is proposed. This procedure, which is quite simple to implement, is outlined in Appendix A. As shown by the examples in the next section, although none of the solutions obtained has been proven to be globally optimal, they are indeed very satisfactory in terms of establishing good targets and comparing very well with literature values.

It should also be noted that in the proposed formulations, the number of stages, NOK, does not necessarily have to be selected as the maximum number of hot or cold streams. Higher values will in general lead to lower estimates of the area although the differences are usually small (see Example 1).

Finally, the formulation for simultaneous energy and area targeting (NLP1) can also be considered as a synthesis model since the solution will indeed define a network configuration which has minimum cost based on area and energy considerations. The other major cost that it does not consider is that of fixed charges for heat exchangers. These charges will be explicitly accounted for in Part II (Yee and Grossmann, 1990) of this series of papers. However, by specifying a fractional exponent for the area cost in the objective function, the model will tend to determine designs requiring minimum number of units in order to take advantage of the economy of scale for the area cost. Therefore, even though the model may not explicitly account for all the cost trade-offs, the solution can lead to near-optimal networks or at least to good starting points for achieving the final network design.

In the next section, examples are presented to illustrate the capabilities of the proposed targeting models. In Examples 1 and 2, the area targeting model corresponding to formulation (NLP2) is used to determine targets for two problems where the utility requirement is fixed. In Examples 3 and 4, the utility requirements for the problems in Examples 1 and 2 are relaxed and, the simultaneous energy and area targeting model corresponding to (NLP1) is applied to account for trade-offs between energy and area costs to determine simultaneously targets for utility consumption and area.

TARGETING EXAMPLES

Example 1

This example is taken from Colberg and Morari (1990). The problem involves two hot streams and two cold streams along with hot and cold utility. Also specified is a heat recovery approach temperature (HRAT) of 10 K, which corresponds to minimum hot and cold utility requirements of 620 and 230 kW, respectively. The data are presented in Table 1. It is interesting to note that the heat transfer coefficients of the streams may differ by an order of magnitude. Since $\max\{N_H, N_C\} = 2$, a two-stage

Table 1. Problem data for Example 1

Stream	TIN (K)	$TOUT$ (K)	Fcp (kW K^{-1})	h (kW m^{-2} K^{-1})	Cost ($ kW-yr^{-1})
H1	395	343	4	2.0	—
H2	405	288	6	0.2	—
C1	293	493	5	2.0	—
C2	353	383	10	0.2	—
S1	520	520	—	2.0	80
W1	278	288	—	2.0	20

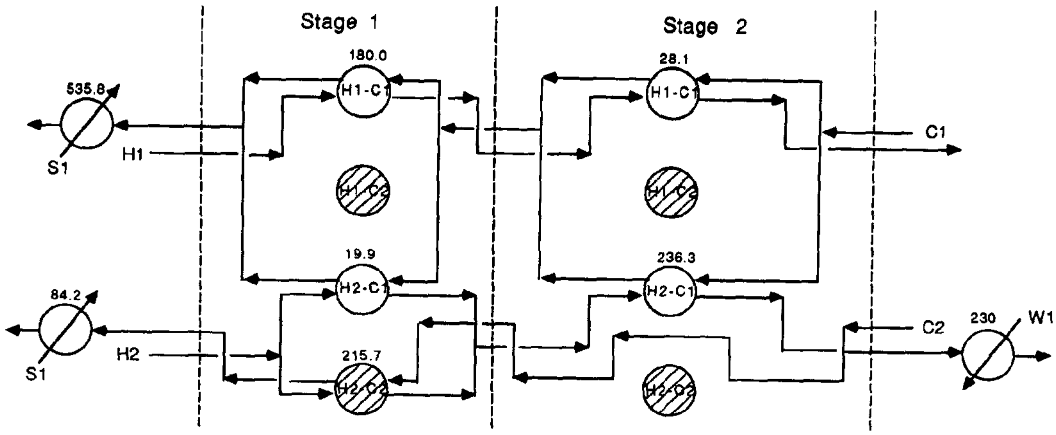

Fig. 4. Example 1 feasible network achieving area target.

NLP formulation corresponding to (NLP2) was set up and solved. The model involved 35 constraints and 25 variables and was solved in 2.6 s on an IBM 3083 using MINOS (Murtagh and Saunders, 1985) via GAMS (Brooke et al., 1988). The solution indicated an area target of 263.6 m^2. The feasible network achieving this target involves eight exchangers and the corresponding network configuration relative to the superstructure is shown in Fig. 4.

As indicated in the remarks section, there is the flexiblity in the model for selecting the number of stages to be used in the superstructure. Typically, the use of $\max\{N_H, N_C\}$ stages will provide a good solution which aside from not requiring large computational time, will generally be closer to the actual area of the final network. A higher number of stages, though, embeds more structures in the representation thus allowing for more opportunities for rematching streams and using more exchangers. However, the expense is that more equations and variables are needed to model the superstructure and solution time will increase. The reverse is true for decreasing the number of stages in the model.

To illustrate the effect of having different number of stages in the superstructure, a three-stage model was also formulated and solved. The formulation contained 43 constraints and 33 variables. Due to its larger size, the solution time of 3.8 CPU s was higher compared to the two stage model (2.6 s). The solution, however, did not differ by much. The three stage model indicated a slightly lower area target of 259.1 m^2 (vs 263.6 m^2) requiring nine exchangers. The two target solutions differ by less than 2%. For this problem, thus, the use of a two-stage representation is certainly adequate.

The two solutions obtained also compare very well with the target from the NLP transshipment model by Colberg and Morari (1990) of 258.8 m^2. As Colberg and Morari noted, if the simple equation by Townsend and Linnhoff (1984) was used, the target would have been 295.6 m^2. This is 14% higher than the solution obtained by the proposed method of this paper.

Design restrictions can also be easily incorporated into the model by fixing or setting bounds on selected variables. If, in the example, a match is forbidden between H1 and C1, heat load variables q_{11k} can be fixed to zero to reflect this requirement. Solving the model with this restriction yielded an area target of 317.8 m^2, which, as expected, is higher than the unrestricted case.

The proposed model has also been used to calculate area targets for other examples reported by Colberg and Morari (1990). To further analyze the effect of changing the number of stages in the proposed representation, the examples were solved first with a formulation with $\max\{N_H, N_C\}$ stages, and then the examples were solved again with one additional stage added to the representation. All the results are presented in Table 2. Targets derived by the Townsend and Linnhoff method are also listed for comparison.

Table 2. Area targeting results comparison

Example	Range of heat transfer coefficients	Townsend and Linnhoff (1984)	Colberg and Morari (1990) solution	Proposed model solution $\max(N_H, N_C)$ stages	Proposed model solution $\max(N_H, N_C)+1$ stages
1	0.2–2.0	295.6	258.8	263.6	259.1
2	0.04–2.0	47.69	29.8	31.3	31.3
3	0.05–3.50	205.6	173.6	179.9	175.5
4	all $h = 0.1$	2896	2896	2898.9	2897.7

Area shown in m^2.
$h = \mathrm{kw\ m^{-2}\,k^{-1}}$

Table 3. Problem data for Example 2

Stream	*TIN* (°F)	*TOUT* (°F)	*Fcp* (kB.t.u. h-°F^{-1})	Cost [\$ yr^{-1} – (kB.t.u. h^{-1})]
H1	320	200	16.67	—
H2	480	280	20.00	—
H3	440	150	28.00	—
H4	520	300	23.80	—
H5	390	150	33.60	—
C1	140	320	14.45	—
C2	240	431	11.53	—
C3	100	430	16.00	—
C4	180	350	32.76	—
C5	200	400	26.35	—
S1	456	456	—	11.05
W1	100	180	—	5.31

$U = 0.15 \dfrac{\text{kB.t.u.}}{\text{h ft}^2\ {}^\circ\text{F}}$

As compared to the results from Colberg and Morari, the proposed model determined very similar area targets although consistently sightly higher in value. Note, however, the difference usually becomes smaller when the number of stages increases. In addition, it should be noted that the higher values can also be attributed to the different LMTD approximations used in the models. Colberg and Morari utilized the Paterson approximation which tends to underestimate the area requirement while the proposed model used the Chen approximation which tends to overestimate the area requirement. Also, it should be noted that for Example 3 from Colberg and Morari (1990), a local solution was obtained for the $\max\{N_H, N_C\}$ case using the proposed initial values of Appendix A. However, after slight modifications on the initial values and resolving the problem, the indicated solution, which is very close to the Colberg and Morari solution, was obtained. Finally, note that for all the cases where the streams have different heat transfer coefficients, the Linnhoff and Townsend targets are significantly higher.

Example 2

This example involves the well-studied 10SP1 problem from Pho and Lapidus (1973). The problem involves 5 hot and 5 cold process streams. The specified level of energy recovery (HRAT = 20°F) corresponds to that of a threshold case where only cold utility is needed. The problem data are presented in Table 3. Note that in this example, all streams have the same heat transfer coefficient.

The proposed model with five stages requires 141 constraints and 196 variables. The optimal solution was obtained after 15.6 CPU s on an IBM 3083. The results indicate an area target of 2490 ft^2 spread over 23 exchangers. Since the heat transfer coefficients for all the streams are the same in this problem, the target using the Townsend and Linnhoff formula is comparable at 2470 ft^2.

Example 3

In the problem of Example 1 in the previous section, an area target was determined based on a fixed level of energy recovery. In this example, the utility requirement is relaxed and energy and area targeting is performed simultaneously. To do so, the objective function is modified to minimize combined annual cost of utilities and area. Utility costs are presented in Table 1. Annual area cost is charged on a per unit area basis of \$200 m^{-2} yr^{-1}. A two-stage representation of the proposed model was used involving 33 constraints and 25 variables. A total CPU time of about 2 s on an IBM 3083 was required to determine the optimal solution. The solution targets an annual cost of \$99,390 yr^{-1}. This comprises a hot utility target of 721.9 kW, a cold utility target of 331.9 kW and an area target of 175 m^2. This level of heat recovery corresponds to an HRAT of roughly 20 K. It is interesting to note that for the same cost for utilities and area, the area targeting solution from the previous section, where HRAT was fixed at 10 K, would yield a combined utility and area annual cost of \$106,140, roughly 7% higher.

To analyze the trade-off between energy and area cost, one can vary the cost of utility and area in the objective function. Tables 4a and b show, respectively, the results from the proposed model when area

Table 4. Target variations with cost

Area cost (\$ m^{-2}-yr^{-1})	Energy and area cost target (\$ yr^{-1})	Hot utility target (kW)	Cold utility target (kW)	Area target (m^2)
(a) Varying area cost for unrestricted case				
100	79,850	651.7	261.7	224.8
200	99,390	721.9	331.9	175.0
300	115,730	772.6	382.6	154.2
Hot utility cost = \$80 (kW-yr^{-1})				
Cold utility cost = \$20 (kW-yr^{-1})				
(b) Varying hot utility cost for unrestricted case				
80	99,390	721.9	331.9	175.0
110	120,590	692.9	302.9	191.6
140	140,040	672.1	282.1	206.6
Area cost = \$200 (m^2-yr^{-1})				
Cold utility cost = \$20 (kW-yr^{-1})				
(c) Varying area cost for restricted case				
100	83,780	675.5	285.5	240.3
200	104,500	754.8	364.8	184.1
300	121,170	806.1	416.1	161.2

Hot utility cost = \$80 (kW-yr^{-1}).
Cold utility cost = \$20 (kW-yr^{-1}).
Match H1–C1 forbidden.

and hot utility costs are varied independently. In Table 4a, area cost is varied from \$100 to \$300 $m^{-2}\,yr^{-1}$. As area cost increases, hot and cold utility costs increase to reduce the amount of area required. In Table 4b, hot utility cost is varied from \$80 to \$140 kW-yr^{-1}. Similar to the trend for area, as utility cost increases, a higher level of energy recovery occurs at the expense of higher area requirement.

The same analysis can be performed for constrained cases previously presented in Example 1. For the case when match H1–C1 is forbidden and for an area cost of \$200 $m^{-2}\,yr^{-1}$, the model predicts an annual energy and area cost of \$104,500 comprising of \$67,680 for utility cost and \$36,820 for area cost. In Example 1, where HRAT was fixed at 10 K, the solution requires an annual energy and area cost of \$117,760 with \$54,200 for utility cost and \$63,560 for area cost. This corresponds to a 13% higher cost target as compared to the simultaneous targeting solution. For completeness, Table 4c provides a study of annual energy and area cost targets for varying per unit area cost for the restricted case. As expected, compared to the nonrestricted case, the cost targets are strictly higher.

Example 4

The 10SP1 problem of Example 2 in the previous section is extended here to target simultaneously for energy and area cost. Costs for utilities are presented in Table 3. The annualized area cost for the problem as given in Pho and Lapidus (1973) is $35 \times (\text{AREA})^{0.6}$ where area is in ft^2. The proposed model with a five-stage representation required 101 constraints and 126 variables. As indicated before, since a fractional exponent was used in the area cost equation, the effect of economy of scale will tend to minimize the number of units although the possibility of local solutions increases due to the nonconvex nature of the function. Using the initialization procedure of the Appendix, the network shown in Fig. 5a was obtained with a computational requirement of 85.7 CPU s on a VAX 6420. This network requires only 10 exchangers and the level of energy recovery corresponds to the threshold case where only cold utility is required and maximum integration is achieved. The annual cost for the network is \$44,560 yr^{-1}, comprising of \$10,040 capital cost and \$34,520 cooling utility cost. Several other starting points were selected and one lead to the network as shown in Fig. 5b with an annual cost of \$43,878. It is interesting to note that this network is the same (except for very small differences in the temperatures of the two split streams) as the one derived by Floudas and Ciric (1989), which is claimed to be the best solution in the literature. It is encouraging to note that even for such a large problem, very good solutions were obtained requiring modest computational times.

MULTI-STREAM HEAT EXCHANGERS

In this section, the proposed heat integration model is used for the design of multi-stream heat exchangers. A single multi-stream heat exchanger can transfer heat between many individual hot and cold streams simultaneously. As a result, accomplishing the many heat transfer tasks in a single unit can lead to substantial savings in both cost and space (Kao, 1961). This is especially relevant in cryogenic processes where equipment have to be kept compact and well insulated. Furthermore, the driving forces are usually low (Fan, 1966). One study done by Edwards and Stinchcome (1977) concluded that plate heat exchangers (where multiple duties can be accomplished) can be very favorable in terms of cost compared to conventional shell and tube exchangers even though they are more limiting in the regions of operation. This is especially true when a special material of construction is required. Also, Lawry (1959) noted that plate exchangers can have very high heat transfer coefficients since the plate arrangements cause turbulent flow even at low fluid velocities.

Typically, for a multi-stream exchanger, there exists a high flexibility in the arrangement of the flows of streams through the exchanger. As a result, the flow arrangement can be configured in the exchanger to favor the maximization of driving forces or the minimization of area requirement. This is illustrated in Fig. 6. For a set of streams with the same heat transfer coefficients, one can arrange the flow pattern to follow the path of the composite curves in order to achieve vertical heat transfer. As indicated in the figure, the inlet and outlet locations of the streams can be strategically located along the exchanger so as to correspond to the kink locations on the composite curves. Using this idea along with the assumption that all the streams have similar temperatures along the exchanger as those on the composite curves, one can reasonably predict the area of the multi-stream exchanger through an area targeting scheme. For cases where the heat transfer coefficients of the streams are not the same, a similar idea can be implemented where inlet and outlet locations are now placed accordingly to allow for certain favorable criss-cross heat transfer.

From the discussion above, the proposed model (NLP2) for area targeting can be easily extended to model multi-stream exchangers. As mentioned previously, the model can account accurately for differences in heat transfer coefficients between the streams. Furthermore, it should be emphasized that the solution obtained, which predicts the area requirement for the multi-stream exchanger, can be very useful in determining the proper flow configuration for the exchanger. This is in view that one can try to mimic the configuration of the solution within the exchanger.

The proposed NLP representation can be embedded into any synthesis or optimization formulation

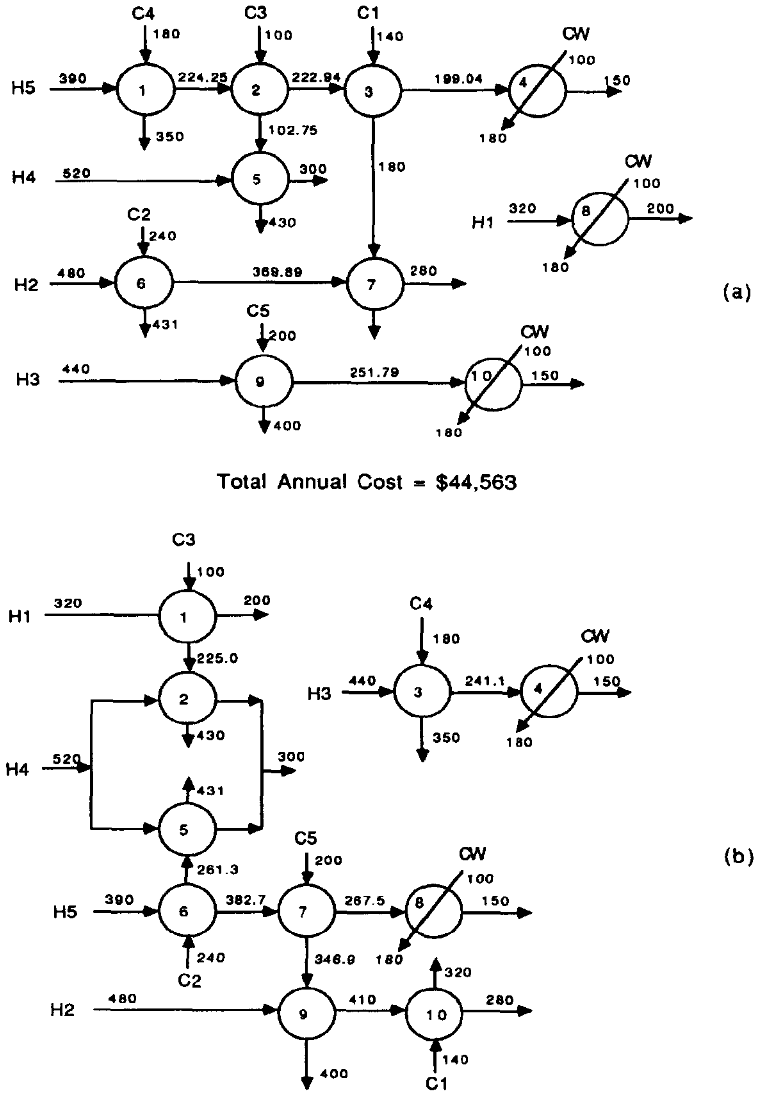

Fig. 5. Networks for the 10SP1 problem.

for fixed network topology to model multi-stream exchangers. Unlike the previous targeting formulations, utilities are not involved and the flows and inlet and outlet temperatures may not necessarily be fixed, but may have to be represented as variables in the model. This means that for equations (1) and (2), the fixed flow parameter F needs to be replaced by the flow variable f. Also, since the inlet and outlet temperatures of the streams to and from the exchanger may not be fixed, the parameters TIN and $TOUT$ may be replaced by inlet temperature variable tin and outlet temperature variable $tout$. With these modifications, constraints for modeling the multi-stream exchangers include equations (1–4) with the cost of the exchanger as its contribution to the overall synthesis objective function. Note that constraints (1) and (2) become nonlinear if the flows are variables. In the example below, an MINLP synthesis model which embeds the proposed representation is used for modeling a multi-stream exchanger.

Example 5

In this example, the proposed model is used to represent a multi-stream heat exchanger which enables a proper account of the trade-offs between the use of multistream heat exchanger and single-hot–single-cold heat exchangers. The problem involves one hot and two cold streams. The data are presented in Table 5. Different cost equations are used for the different types of exchangers. For

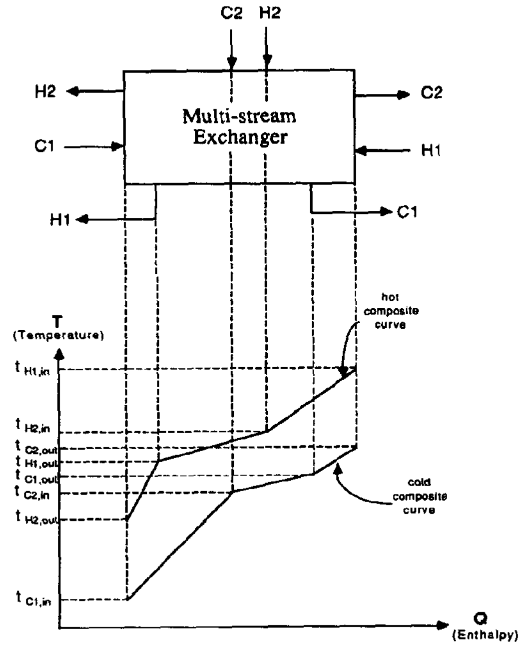

Fig. 6. Representation of multi-stream exchanger on composite curves.

the multi-stream exchanger, the fixed charge is significantly higher and the area cost is on a per unit basis (Usher, 1983). Also, the heat transfer coefficients for the multi-stream exchangers are 10% higher.

The formulation for the problem is based on the superstructure representation of Yee and Grossmann (1988) as shown in Fig. 7. Two exchangers are shown in the superstructure and can be used for any of the possible matches. However, exchanger 2 is modified to embed both the possibility of a single-hot–single-cold exchanger or a multi-stream exchanger serving both cold streams. Since fixed charges are explicitly involved, the model formulation becomes a mixed integer nonlinear programming problem. Structural decisions are, therefore, determined by the use of binary variables. Also, in the formulation, nonsmooth terms are eliminated through the use of the binary variables and the introduction of approach temperature variables. More detailed discussion of this representation is given in Part II of this series of papers (Yee and Grossmann, 1990).

Table 5. Problem data for Example 5

Stream	*TIN* (K)	*TOUT* (K)	*Fcp* ($kW\,K^{-1}$)
H1	420	370	8
C1	300	350	4
C2	280	320	5

Single-hot–single-cold exchangers:
$U = 1\ kW\,m^{-2}\,K^{-1}$ for all matches
Exchanger cost = $8600 + 670 \times (\text{Area})^{0.83}$

Multi-stream exchangers:
$U = 1.1\ kW\,m^{-2}\,K^{-1}$ for all matches
Exchanger cost = $15{,}000 + 400 \times (\text{Area})$

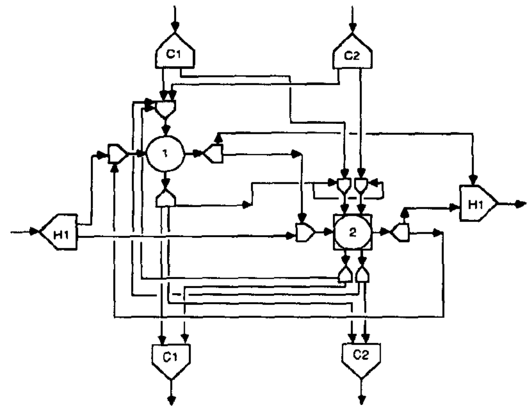

Fig. 7. Superstructure for Example 5.

In the formulation, a two-stage representation was used to model the multi-stream exchanger. The overall formulation involves 61 constraints and 61 variables. The model was solved using DICOPT++ (Viswanathan and Grossmann, 1990) with MINOS (Murtagh and Saunders, 1985) and MPSX (IBM, 1979). Part II (Yee and Grossmann, 1990) provides a brief discussion of the algorithm. Three major iterations were required using a total CPU time of 8.7 s on an IBM 3083. The solution obtained identified that the use of a single multi-stream exchanger is more cost-effective than using two conventional single-hot–single-cold exchangers. The selected network configuration is shown in Fig. 8. The capital cost required is $32,710. For comparison, if two conventional exchangers are used instead, the best solution that can be achieved requires a capital cost of $36,440, which is about 11% higher.

CONCLUSION

In this paper, a superstructure for heat integration problems has been introduced which does not require the definition of temperature or enthalpy intervals. This superstructure has been applied to energy and

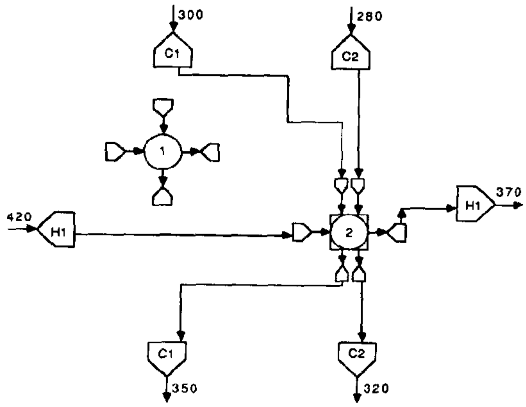

Fig. 8. Optimal network for Example 5.

area targets, and to the modeling of multi-stream heat exchangers, in order to account simultaneously for the different trade-offs without requiring the use of common heuristics.

The model (NLP2) was first applied to the HEN area targeting problem. As illustrated by the examples, the model can properly account for the differences of heat transfer coefficients amongst the streams. Results have compared very well with available literature values. In addition, the solution of the problem will always provide a feasible network including its configuration. By relaxing the utility consumption specified in the area targeting formulation and modifying the objective function to account for cost utilities as well as area, the model (NLP1) can simultaneously target for energy as well as area. Examples have shown that the model can properly account for the trade-offs between the costs. Computationally, the advantage of the two proposed models (NLP1) and (NLP2) is that since they only involve linear constraints, the solutions can be obtained quite efficiently as shown by the example problems. The potential limitation is that these models can have multiple local solutions. The proposed initialization procedure, however, has shown to perform well although it cannot of course guarantee global optimality.

Finally, the model was applied for the design of multi-stream heat exchangers. In this case, flows become variables and the model predicts an area target for the multi-stream heat exchanger involving the selected streams serviced. In general, this is a good approximation since sufficient flexiblity in the flow arrangement in the multi-stream exchanger can usually achieve minimal area requirement. This model can be embedded in any synthesis problem to represent a multi-stream heat exchanger. An example was presented to show that trade-offs between selecting single-hot–single-cold exchangers vs multi-stream exchangers can be properly modeled.

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APPENDIX

Initialization Procedure for Solving the NLP Models

In this paper, NLP models were proposed for simultaneous area and energy targeting based on cost and for a fixed level of energy recovery, area targeting. Although these models have strictly linear feasible regions, nonlinearities in the objective function terms which calculate the area requirement for the exchangers, are nonconvex in nature. This nonconvexity, as a result, may cause the model to have more than one local optimal solution. Therefore, to increase the probability of obtaining the globally optimal solution, a good initialization strategy may be required.

The initialization scheme proposed here is a simple one. The strategy is to provide reasonable initial values to favor the minimization of the various costs involved. The notations for the equations below follow the nomenclature presented earlier. Also, the expression $.I$ following the variable represents the initialization for the particular variable.

First, the temperatures variables are bounded and initialized to that they provide a high driving force for the exchangers to minimize area:

$$
\begin{aligned}
&t_{ik} \leqslant TIN_i, \quad t_{ik} \geqslant TOUT_i \qquad i \in HP, \quad k \in ST, \\
&t_{jk} \leqslant TOUT_j, \quad t_{jk} \geqslant TIN_j, \qquad j \in CP, \quad k \in ST, \\
&t_{ik}.I = TIN_i, \qquad i \in HP, \quad k \in ST, \\
&t_{jk}.I = TIN_j, \qquad j \in CP, \quad k \in ST. \qquad \text{(A1)}
\end{aligned}
$$

Next, the heat load for each exchanger can be initialized to a value which spreads out the heat transfer amongst the NOK number of stages. Note that in the following, the maximum heat transfer for a particular pair of hot and cold stream is the minimum of either the hot or the cold stream heat loads:

$$q_{ijk}.I = \min[F_i(TIN_i - TOUT_i), F_j(TOUT_j - TIN_j)]/NOK,$$
$$i \in HP, \quad j \in CP, \quad k \in ST.$$

Finally, the variables for hot and cold utility loads can be initialized to small values so as to favor the minimization of the utility costs. For the area targeting case, though, where the utility requirement is fixed, these variables can be initialized to evenly distribute the required utility heat loads amongst the streams. Although the above strategy is quite simple, it has provided very good results in the examples presented.