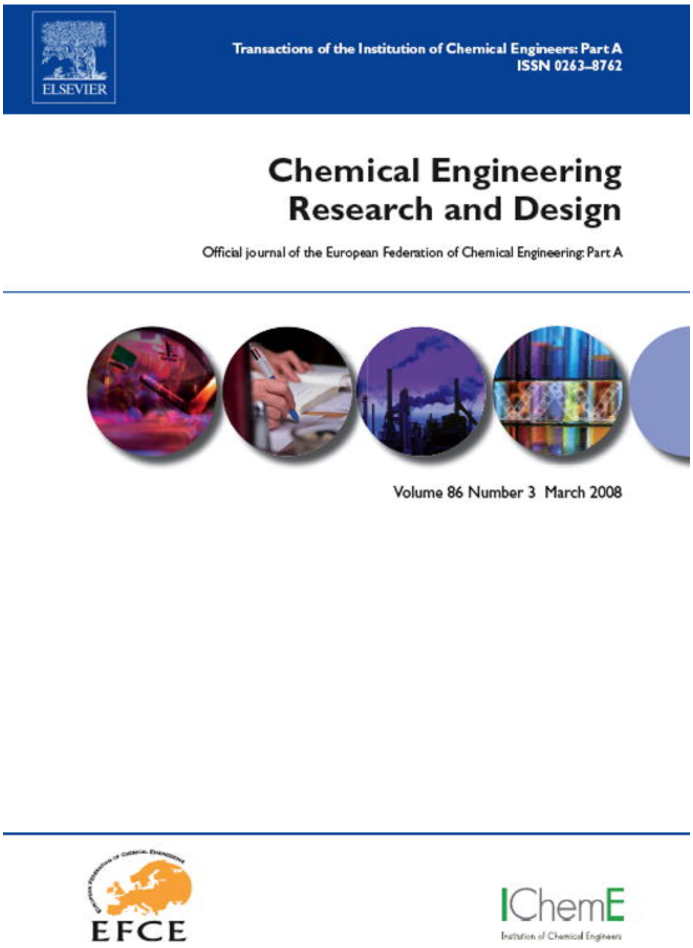

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Simultaneous optimization strategy for synthesizing heat exchanger networks with multi-stream mixers

Hong-Guang Dong[a], *Chih-Yao Lin*[b], *Chuei-Tin Chang*[b,*]

[a] *School of Chemical Engineering, Dalian University of Technology, Dalian 116012, Liao Ning, PR China*
[b] *Department of Chemical Engineering, National Cheng Kung University, Tainan 70101, Taiwan, ROC*

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ABSTRACT

A systematic procedure is proposed in this paper to incorporate the options of merging and/or splitting process streams from *multiple origins* in heat exchanger network (HEN) design. The utility and capital costs of a traditional HEN may both be reduced significantly with this practice since: (1) the direct heat-exchange operations are more efficient thermodynamically, (2) the mixers are in general less expensive than the indirect heat-transfer units, and (3) the matches between hot and cold streams can be more appropriately placed by taking advantage of the added structural flexibility. A state-space concept is adopted in this work to construct a superstructure for capturing the characteristics of network configuration. More specifically, any HEN (with or without multi-stream mixers) is viewed as a collection of two interconnected blocks, i.e., the process operator and the distribution network. A mixed integer nonlinear program (MINLP) is then formulated accordingly for one-step minimization of the total annualized cost. Based upon the proposed stochastic initiation strategy and solution clustering method, an efficient algorithm is developed to obtain the global optimum of this MINLP model with high creditability. Several examples are also presented to demonstrate the feasibility and benefits of the proposed approach.

1. Introduction

Heat exchanger network design is an essential element in devising the energy management system of any chemical process plant. A large volume of related studies have already been published in the literature. Basically, two distinct approaches were adopted in these works: (a) the heuristics-based Pinch design method (Linhoff and Hindmarsh, 1983) and (b) the model-based optimization method (Papoulias and Grossmann, 1983; Ciric and Floudas, 1991). All of them were developed by maintaining the identity of every process stream in HEN design. However, in many existing chemical processes, multiple hot and/or cold streams may be allowed to be merged before entering the same unit or splitting again for different processes. For example, the overhead product streams of a multi-effect distillation unit might be combined and then cooled (or heated) to the operating temperature of a downstream unit; naphtha and hydrogen may be merged and heated to the reaction temperature in the hydrotreating plant of a refinery; the various heating (or cooling) utilities in a chemical plant may also be mixed and distributed in a pipeline network. Notice also that this practice becomes even more attractive if multiple water streams are involved. For example, the wastewaters within a process could be collected and then distributed to various treatment units before disposal. These waters may be originated from different production units at different temperatures. Since there is no need to maintain a finite temperature approach in a direct heat exchanger and the mixer is much cheaper than a traditional heat exchanger, it is reasonable to expect that the capital costs of HEN can be drastically reduced by incorporating the multi-stream mixing/splitting options. A Pinch-analysis based HEN design approach has already been developed by Savulescu et al. (2002) to take advantage of this additional design flexibility in integrating water and energy networks.

In a preliminary study, Chang and Yu (1988) showed that the design practices of mixing hot with hot streams (or cold with cold streams) can be used in an evolutionary synthe-

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[*] Corresponding author. Tel.: +886 6 275 7575x62663; fax: +886 6 234 4496.
E-mail addresses: donghg@mail.ncku.edu.tw (H.-G. Dong), ctchang@mail.ncku.edu.tw (C.-T. Chang).

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Nomenclature

$A_{i,j}$	the heat-transfer area in an heat exchanger between the ith hot stream and jth cold stream.
$f_{p,q,r}$	product of heat capacity and mass flow rate associated with a branch from the splitter on the qth hot or cold stream entering from environment ($p=1$) and from OP block ($p=2$), respectively to the rth outlet mixer
$F_{p,i}^{IN}$, $F_{p,j}^{IN}$	the products of heat capacity and mass flow rate of the ith hot stream and jth cold stream entering DN block from environment ($p=1$) and from OP block ($p=2$), respectively.
$F_{p,i}^{OUT}$, $F_{p,j}^{OUT}$	the products of heat capacity and mass flow rate of the ith hot stream and jth cold stream leaving from DN block to the OP block ($p=1$) and to the environment ($p=2$), respectively.
k	counter of algorithm iteration of generation feasible solutions sample
K_{seed}	the number of optimal solutions after cluster identification
$K_{perturb}$	the upper bound number of termination algorithm iteration of lth optimal solution variables perturb
K_{target}	the upper bound number of termination algorithm iteration of generation feasible solutions sample
l	ordinal of optimal solutions after cluster identification
m	counter of algorithm iteration of the real and binary variables perturb
m, n	the numbers of interior junctions associated with hot streams and cold streams in general.
m_i, n_j	the numbers of interior junctions associated with exterior hot stream i and exterior cold stream j, respectively.
M_{ext}, N_{ext}	the numbers of exterior junctions on the DN block for the hot and cold streams, respectively from (or to) the environment.
M_{int}, N_{ext}	the numbers of interior junctions on the DN block for the hot and cold streams, respectively from (or to) the OP block.
M_p^{IN}, N_p^{IN}	the numbers of inlet splitters for hot and cold streams on the DN block from environment ($p=1$) and from OP block ($p=2$), respectively.
M_p^{OUT}, N_p^{OUT}	the numbers of outlet mixers for hot and cold streams on the DN block to the OP block ($p=1$) and to the environment ($p=2$), respectively.
T_i^{in}, T_i^{out}	the hot stream temperatures at the inlet and outlet of exchanger (i, j), respectively.
T_j^{in}, T_j^{out}	the cold stream temperatures at the inlet and outlet of exchanger (i, j), respectively.
$T_{p,i}^{IN}$, $T_{p,j}^{IN}$	the temperatures of the ith hot stream and jth cold stream entering DN block from environment ($p=1$) and from OP block ($p=2$), respectively.
$T_{p,i}^{OUT}$, $T_{p,j}^{OUT}$	the temperatures of the ith hot stream and jth cold stream leaving from DN block to the OP block ($p=1$) and to the environment ($p=2$), respectively.
ΔT_{min}	the minimum temperature approach.
$\Delta \bar{T}_{i,j}$	the log-mean temperature difference in the exchanger (i, j).
$U_{i,j}$	the overall heat-transfer coefficient of exchanger (i, j).
$z_{i,j}$	the binary variable reflecting whether or not the match between streams i and j exists

Greek letters

δ	the range of perturbation interval
$\varepsilon_{p,q,r}$	the randomly generated perturbation for $\varphi_{p,q,r}$.
$\varphi_{p,q,r}$	the split ratio of a branch leaving the splitter on the qth hot (or cold) stream entering the DN block from environment ($p=1$) and from OP block ($p=2$), respectively to the rth mixer leaving the DN block.
Γ_H, Γ_C	the sets of hot and cold streams entering the OP block.

Subscripts

ext	external
int	internal

Superscripts

in	exchanger inlet
out	exchanger outlet
IN	DN inlet
OUT	DN outlet

sis procedure to reduce the number of heat exchangers in a maximum energy recovery network without energy penalty. In another study performed by Chang et al. (1994), it was demonstrated that the capital costs of HENs could be lowered significantly without increasing the operating costs by considering the aforementioned mixing options. The proposed design procedure was carried out sequentially in three steps: (1) solve a linear programming (LP) model to determine the minimum consumption rates of utilities, (2) solve a mixed integer linear programming (MILP) model to determine the minimum number of matches and the corresponding heat duties, (3) solve a nonlinear programming (NLP) model to obtain a cost-optimal network. This approach is quite effective for obtaining a feasible (but may be suboptimal) solution since the three decomposed optimization problems are smaller and therefore more tractable. Chang and Chen (1997) later suggested that mixing the hot and cold streams can be viewed as an alternative means of heat exchange without the need for enforcing a nonzero minimum temperature approach. A similar sequential design procedure was also developed. The main contribution of this work is a two-scale temperature partition scheme. Specifically, the temperature range of all process streams is partitioned into K intervals according to two different ΔT_{min} s. A value of zero is used for mixers, while a positive ΔT_{min} is adopted as the lower limit of driving force in a conventional heat exchanger. It was concluded that the proposed approach can be used to cut down not only the capital investments but also the utility consumption rates of heat recovery systems.

It is obvious that the HEN design obtained with the aforementioned sequential procedure may not be truly optimal. This is due to the fact that the trade-offs between the consecutive optimization steps are ignored. A simultaneous solution strategy is therefore needed to circumvent this drawback. To this end, Yee et al. (1990) and Yee and Grossmann (1990) proposed a stage-wise superstructure and formulated a MINLP model accordingly for synthesizing the heat exchanger networks with a simultaneous optimization procedure. However, it is very difficult to incorporate various stream mixing/splitting options with their general network configuration since the material balances were not adopted as model constraints. On the other hand, Papalexaddri and Pistikopoulos (1994) developed a hyperstructure to universally represent all possible process alternatives with a multipurpose block. A multi-period MINLP model can be constructed accordingly for heat- and mass-exchange network synthesis. Although this approach is quite effective for conventional HEN design, it is not very convenient to produce the matrix expressions needed for the present applications. The state-space concept (Bagajewicz and Manousiouthakis, 1992; Bagajewicz et al., 1998) is thus adopted in the present study to construct a superstructure for capturing the special features of a generalized HEN which allows direct heat exchanges between process streams. This modified state-space representation and the corresponding MINLP model are described in the following section. A two-stage optimization algorithm is presented in Section 3. In particular, a stochastic initialization mechanism and a clustering procedure are first utilized to identify the most possible solution region. A detailed search strategy is then applied in the second stage to locate the true optimum. Three examples are presented in Section 4 to show the feasibility and effectiveness of the proposed simultaneous optimization strategy. The benefits of installing multi-stream mixers in HEN are also clearly demonstrated in the results given in the case studies. Finally, the conclusions of present works and some comments on future studies are provided in Section 5.

2. The state-space models

The state-space superstructure was first proposed by Bagajewicz and Manousiouthakis (1992) as an alternative representation of the HEN configuration. This original structure has been modified in the present work to incorporate *direct* heat exchange as a design option. Specifically, the HEN is viewed as a system of two interconnected blocks (see Fig. 1). One is referred to as the distribution network (DN), in which all mixers, splitters and the connections between them are embedded. The other is the so-called process operator (OP), in which all *indirect* heat exchanges in HEN take place. The detailed configurations and the corresponding mathematical models of these two blocks are outlined in the sequel.

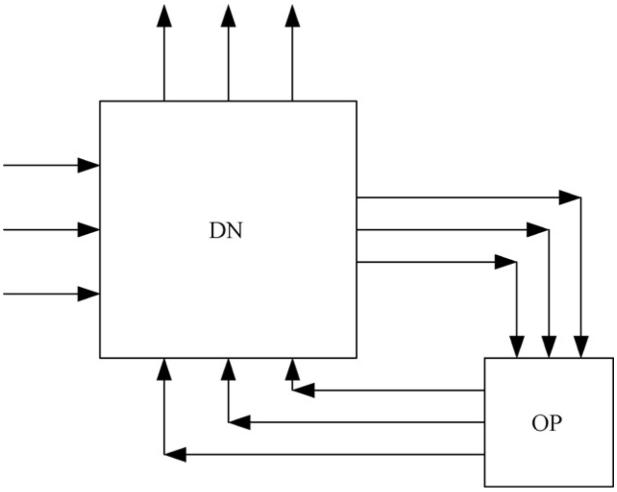

Fig. 1 – General structure of state-space representation.

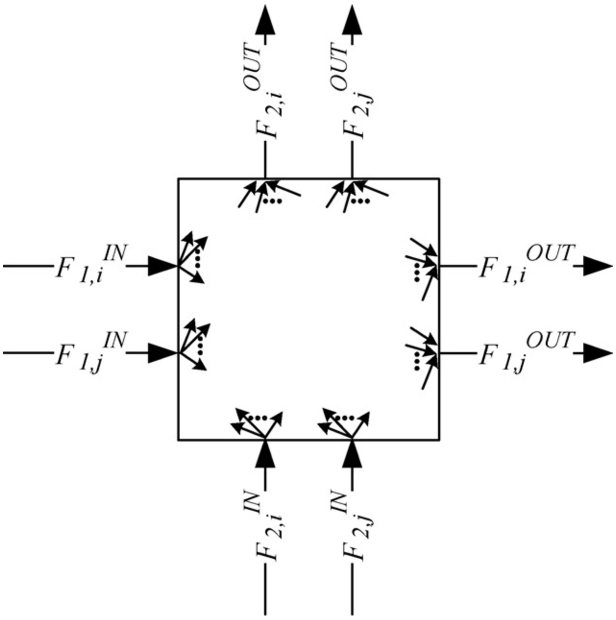

Fig. 2 – General distribution network.

2.1. Distribution network

The configuration of a general DN block is shown in Fig. 2. Here, the indices *i* and *j* denote, respectively a hot and a cold stream. Every entering or recycling stream can be split into several branches and each of them is connected to a mixer at the exit leading to the OP block or environment. The mathematic model of the distribution network is presented as follow:

$$F_{1,i}^{IN} = \sum_{l=1}^{M_1^{out}+N_1^{out}} f_{1,i,l} + \sum_{k=1}^{M_2^{out}+N_2^{out}} f_{1,i,k} \quad i = 1, 2, \ldots, M_1^{in} \tag{1}$$

$$F_{1,j}^{IN} = \sum_{l=1}^{M_1^{out}+N_1^{out}} f_{1,j,l} + \sum_{k=1}^{M_2^{out}+N_2^{out}} f_{1,j,k} \quad j = 1, 2, \ldots, N_1^{in} \tag{2}$$

$$F_{1,i}^{OUT} = \sum_{k=1}^{M_1^{in}} f_{1,k,i} + \sum_{l=1}^{N_1^{in}} f_{1,l,i} + \sum_{k=1}^{M_2^{in}} f_{2,k,i} + \sum_{l=1}^{N_2^{in}} f_{2,l,i} \quad i = 1, 2, \ldots, M_1^{out} \tag{3}$$

$$F_{1,i}^{OUT} T_{1,i}^{OUT} = \sum_{k=1}^{M_1^{in}} f_{1,k,i} T_{1,k}^{IN} + \sum_{l=1}^{N_1^{in}} f_{1,l,i} T_{1,l}^{IN} + \sum_{k=1}^{M_2^{in}} f_{2,k,i} T_{2,k}^{IN} + \sum_{l=1}^{N_2^{in}} f_{2,l,i} T_{2,l}^{IN}$$
$$i = 1, 2, \ldots, M_1^{out} \tag{4}$$

$$F_{1,j}^{OUT} = \sum_{k=1}^{M_1^{in}} f_{1,k,j} + \sum_{l=1}^{N_1^{in}} f_{1,l,j} + \sum_{k=1}^{M_2^{in}} f_{2,k,j} + \sum_{l=1}^{N_2^{in}} f_{2,l,j} \quad j = 1, 2, \ldots, N_1^{out} \tag{5}$$

$$F^{OUT}_{1,j}T^{OUT}_{1,j}=\sum_{k=1}^{M_1^{in}} f_{1,k,j}T^{IN}_{1,k}+\sum_{l=1}^{N_1^{in}} f_{1,l,j}T^{IN}_{1,l}+\sum_{k=1}^{M_2^{in}} f_{2,k,j}T^{IN}_{2,k}+\sum_{l=1}^{N_2^{in}} f_{2,l,j}T^{IN}_{2,l}$$

$$j=1,2,\ldots,N_1^{out} \tag{6}$$

$$F^{IN}_{2,i}=\sum_{l=1}^{M_1^{out}+N_1^{out}} f_{2,i,l}+\sum_{k=1}^{M_2^{out}+N_2^{out}} f_{2,i,k}\qquad i=1,2,\ldots,M_2^{in} \tag{7}$$

$$F^{IN}_{2,j}=\sum_{l=1}^{M_1^{out}+N_1^{out}} f_{2,j,l}+\sum_{k=1}^{M_2^{out}+N_2^{out}} f_{2,j,k}\quad j=1,2,\ldots,N_2^{in} \tag{8}$$

$$F^{OUT}_{2,i}=\sum_{k=1}^{M_1^{in}} f_{1,k,i}+\sum_{l=1}^{N_1^{in}} f_{1,l,i}+\sum_{k=1}^{M_2^{in}} f_{2,k,i}+\sum_{l=1}^{N_2^{in}} f_{2,l,i}\quad i=1,2,\ldots,M_2^{out} \tag{9}$$

$$F^{OUT}_{2,i}T^{OUT}_{2,i}=\sum_{k=1}^{M_1^{in}} f_{1,k,i}T^{IN}_{1,k}+\sum_{l=1}^{N_1^{in}} f_{1,l,i}T^{IN}_{1,l}+\sum_{k=1}^{M_2^{in}} f_{2,k,i}T^{IN}_{2,k}+\sum_{l=1}^{N_2^{in}} f_{2,l,i}T^{IN}_{2,l}$$

$$i=1,2,\ldots,M_2^{out} \tag{10}$$

$$F^{OUT}_{2,j}=\sum_{k=1}^{M_1^{in}} f_{1,k,j}+\sum_{l=1}^{N_1^{in}} f_{1,l,j}+\sum_{k=1}^{M_2^{in}} f_{2,k,j}+\sum_{l=1}^{N_2^{in}} f_{2,l,j}\quad j=1,2,\ldots,N_2^{out} \tag{11}$$

$$F^{OUT}_{2,j}T^{OUT}_{2,j}=\sum_{k=1}^{M_1^{in}} f_{1,k,j}T^{IN}_{1,k}+\sum_{l=1}^{N_1^{in}} f_{1,l,j}T^{IN}_{1,l}+\sum_{k=1}^{M_2^{in}} f_{2,k,j}T^{IN}_{2,k}+\sum_{l=1}^{N_2^{in}} f_{2,l,j}T^{IN}_{2,l}$$

$$j=1,2,\ldots,N_2^{out} \tag{12}$$

where $F^{IN}_{p,i}$ and $F^{IN}_{p,j}$ represent the products of heat capacity and mass flow rate associated with the ith hot stream and jth cold stream entering DN block from environment ($p=1$) and from OP block ($p=2$), respectively; $F^{OUT}_{p,i}$ and $F^{OUT}_{p,j}$ denote the products of heat capacity and mass flow rate associated with the ith hot stream and jth cold stream leaving from DN block to the OP block ($p=1$) and to the environment ($p=2$), respectively; $f_{p,q,r}$ is the product of heat capacity and mass flow rate associated with a branch from the splitter on the qth hot (or cold) stream entering from environment ($p=1$) and from OP block ($p=2$), respectively to the rth outlet mixer; M_p^{IN} and $N_p^{IN}(p=1, 2)$ represent the numbers of inlet splitters for hot and cold streams, respectively; M_p^{OUT} and $N_p^{OUT}(p=1, 2)$ represent the numbers of outlet mixers of hot and cold streams. Notice that, for a given design problem, the numbers of exterior junctions to and from environment are fixed, i.e., $M_1^{IN}=M_2^{OUT}=M_{ext}$ and $N_1^{IN}=N_2^{OUT}=N_{ext}$ are constants. On the other hand, the numbers of interior junctions to and from the OP block are adjustable parameters, i.e., $M_1^{out}=M_2^{in}=M_{int}$ and $N_{1,j}^{out}=N_{2,j}^{in}=N_{int}$ should be chosen by the designer(s). Consequently,

$$F^{OUT}_{1,i}=F^{IN}_{2,i}=F_i \tag{13}$$

$$F^{OUT}_{1,j}=F^{IN}_{2,j}=F_j \tag{14}$$

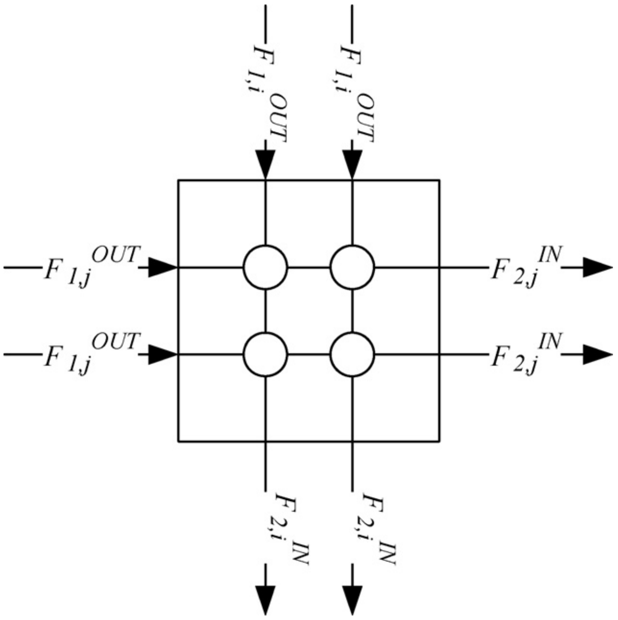

Fig. 3 – Typical process operator.

2.2. *Process operator*

A typical OP block is shown in Fig. 3. Notice first that the energy balance around each exchanger can hold only when the corresponding match is active, i.e.

$$z_{i,j}[F_i(T_i^{in}-T_i^{out})-F_j(T_j^{out}-T_j^{in})]=0\quad i\in\Gamma_H,\quad j\in\Gamma_C \tag{15}$$

where Γ_H and Γ_C represent, respectively the sets of hot and cold streams entering the process operator; $z_{i,j}$ the binary variable reflecting whether or not the match between streams i and j exists; T_i^{in} and T_i^{out} denote, respectively the hot stream temperatures at the inlet and outlet of exchanger (i, j); T_j^{in} and T_j^{out} denote, respectively the cold stream temperatures at the inlet and outlet of exchanger (i, j). The heat transfer area needed for each match can be determined according to the following equation:

$$z_{i,j}[F_j(T_j^{out}-T_j^{in})-U_{i,j}A_{i,j}\Delta\bar{T}_{i,j}]=0\quad i\in\Gamma_H\quad j\in\Gamma_C \tag{16}$$

where $U_{i,j}$ is the overall heat-transfer coefficient; $A_{i,j}$ is the heat-transfer area; $\Delta\bar{T}_{i,j}$ is the log-mean temperature difference in the exchanger. Finally, the hot stream and cold stream temperatures at the inlets and outlets of every exchanger should satisfy the second law of thermodynamics, i.e.

$$z_{i,j}(T_j^{in}-T_i^{out})\le 0\quad i\in\Gamma_H\quad j\in\Gamma_C \tag{17}$$

$$z_{i,j}(T_j^{out}-T_i^{in})\le 0\quad i\in\Gamma_H\quad j\in\Gamma_C \tag{18}$$

$$T_i^{out}-T_i^{in}\le 0\quad i\in\Gamma_H \tag{19}$$

$$T_j^{in}-T_j^{out}\le 0\quad i\in\Gamma_C \tag{20}$$

2.3. *Connecting junctions*

As mentioned previously, the numbers of interior junctions, M_{int} and N_{int}, must be chosen to facilitate satisfactory solution of the state-space model. To address this issue, let us first consider the original model formulation. Notice that, if the process streams in a HEN are *not* allowed to be mixed with one another, then every interior junction can be used for exactly one of them. Bagajewicz et al. (1998) introduced two sets of additional match constraints in their mixed-integer nonlinear program for the purpose of incorporating all possible match sequences in the superstructure, i.e.

$$\sum_{j=1}^{N_{\text{int}}} z_{ij} = 1 \quad i = 1, 2, \ldots, M_{\text{int}} \tag{21}$$

$$\sum_{i=1}^{M_{\text{int}}} z_{ij} = 1 \quad j = 1, 2, \ldots, N_{\text{int}} \tag{22}$$

Thus, in order to provide enough opportunities to match every cold (or hot) stream with a particular hot (or cold) stream, it is imperative to select the numbers of interior junctions according to the criteria listed below:

$$1 \le m_i \le N_{\text{ext}} \quad i = 1, 2, \ldots, M_{\text{ext}} \tag{23}$$

$$1 \le n_j \le M_{\text{ext}} \quad j = 1, 2, \ldots, N_{\text{ext}} \tag{24}$$

where m_i and n_j denote, respectively the numbers of interior junctions associated with exterior hot stream i and exterior cold stream j. Thus, the maximum number of interior junctions should be $2M_{\text{ext}}N_{\text{ext}}$. It is also clear that

$$\sum_{i=1}^{M_{\text{ext}}} m_i = M_{\text{int}} \tag{25}$$

$$\sum_{j=1}^{N_{\text{ext}}} n_j = N_{\text{int}} \tag{26}$$

The optimal HEN can be identified by the selecting the numbers of interior junctions and then solving the corresponding MINLP model in a trial-and-error fashion. The values of m_is and n_js were increased one-at-a-time from their lower limits (Bagajewicz et al., 1998).

In our study, the match constraints (21) and (22) are *omitted*. Notice that none of the network configurations considered in the original formulation is excluded by this practice. The relaxed problem is in fact easier to solve since a feasible optimum may be reached with fewer interior junctions. Eqs. (23) and (24) can still be adopted as conservative estimates of the possible ranges of junction numbers in a *traditional* HEN synthesis problem. However, it is anticipated that an optimal HEN can be obtained with smaller m_is and n_js in the trial-and-error process. On the other hand, if all streams in a HEN are mixable, then the distinction between any two interior junctions vanishes. Consequently, the numbers of interior junctions in this case can be chosen with the following heuristics:

$$0 \le m \le N_{\text{ext}} \tag{27}$$

$$0 \le n \le M_{\text{ext}} \tag{28}$$

$$m + n \ge 1 \tag{29}$$

where m and n denote, respectively the numbers of interior junctions associated with hot streams and cold streams *in general*. Notice that it is possible to construct a superstructure *without* either hot or cold junctions according to these heuristic rules. In such cases, only direct heat exchanges are allowed in HEN. Notice also that the maximum number of interior junctions is now reduced to $M_{\text{ext}} + N_{\text{ext}}$.

Finally, in practical applications, more than one group of mixable process streams may coexist with streams that are not mixable. The aforementioned principles for setting the numbers of interior junctions are still applicable in such scenarios.

3. Solution strategy

Although a large number of deterministic methods for solving the MINLP problems have already been reviewed by Floudas et al. (2005), the aforementioned model still calls for the development of a dedicated solution strategy due to its complexity. By incorporating both deterministic and stochastic components, a hybrid optimization strategy is developed in this work to enhance the solution quality. More specifically, the proposed algorithm can be applied to identify a near global optimum within an acceptable amount of time.

The proposed solution procedure can be divided into two stages. The first is designed to generate a set of initial feasible solutions and then identify the candidate region for refined search, while the second is aimed to locate the true optimum with perturbation techniques. The DICOPT solver (Viswanathan and Grossmann, 1990) in GAMS is used in this study to solve the MINLP models and it is interfaced with MATLAB (Ferris, 2005) for executing various initiation and perturbation steps automatically. The detailed solution steps are given in the flowchart shown in Fig. 4. Notice that this procedure is still required to be carried out repeatedly for various combinations of hot and cold junction numbers. In addition, to implement the proposed solution strategy, the upper and lower utility bounds must be determined in advance. In this work, $Q_h^{\max}$ and $Q_c^{\max}$ are calculated by assuming that all heating and cooling duties of the process streams are satisfied with utilities exclusively. On the other hand, the minimum utility consumption rates are computed with the LP model proposed by Chang and Chen (1997) on the basis of zero minimum temperature approach.

The first step in Stage I is to produce a set of initial guesses of the decision variables with a random number generator. In the MINLP model, these decision variables are chosen to be the binary variables z_{ij}s and also the split ratios of all splitters. The latter variables are defined as

$$\varphi_{p,q,r} = \frac{f_{p,q,r}}{F_{p,q}^{\text{IN}}} \tag{30}$$

where $\varphi_{p,q,r}$ denotes the split ratio of a branch leaving the splitter on the qth hot (or cold) stream entering from environment ($p=1$) and from OP block ($p=2$), respectively to the rth outlet mixer. Notice that Eqs. (1), (2), (7) and (8) can be re-written in a unified format according to this definition:

$$\sum_{l=1}^{M_1^{\text{out}}+N_1^{\text{out}}} \varphi_{p,q,l} + \sum_{k=1}^{M_2^{\text{out}}+N_2^{\text{out}}} \varphi_{p,q,k} = 1 \tag{31}$$

where $p=1, 2$ and $q = 1, 2, \ldots, M_p^{\text{in}}$(or N_p^{in}). The primary objective at this point is to obtain the feasible solution of the original MINLP problem directly with the randomly generated initial

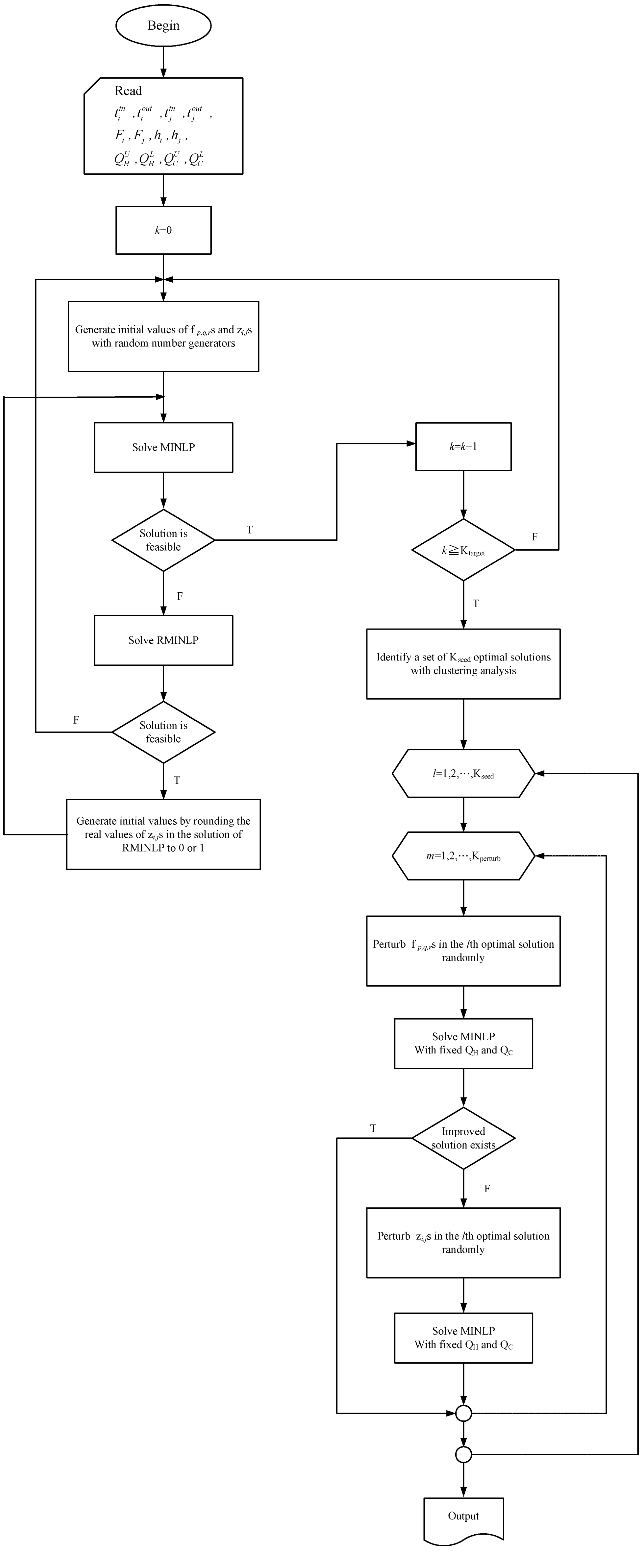

Fig. 4 – Solution strategy.

guesses. If this is not possible, a relaxed MINLP is then solved with the same initial guesses. If this attempt is successful, the solution of RMINLP is then slightly modified to create an additional set of initial guesses for the original MINLP problem. In particular, if a relaxed binary variable is found to be close to 1 (say, larger than 0.7), the corresponding initial value can be set to one. A similar practice can be used to set the initial value of a close-to-zero (say, less than 0.3) binary variable. The other relaxed variables should be left unspecified. However, if the solution process of the RMINLP model is not convergent, the search procedure in Stage I should be restarted by generating another set of initial guesses randomly. The procedure in Stage I is repeated until a predetermined number of feasible solutions can be obtained.

It is well established that the numerical iteration process in solving a MINLP problem is highly dependent upon the initial guesses and may converge to a local optimum. To enhance the solution quality, the *K*-means clustering technique (Kaufman and Rousseeuw, 1990) is adopted to identify a candidate region for further refined search. This technique can be used to partition a collection of given data sets into *K* mutually exclusive clusters. Each cluster is characterized by its centroid. To reduce the computation load, only the objective value and the corresponding hot and cold utility consumption rates in each initial feasible solution are included in a data set for the clustering analysis. In general, 2 or 3 clusters are sufficient for our purpose. The cluster with the lowest (or highest) objective value at its centroid is selected as the candidate region.

During the second stage, new initial guesses are created by introducing random perturbations into the initial feasible solutions which are in the immediate neighborhood of the centroid in the candidate region. More specifically, the initial split ratios are adjusted according to the following equation:

$$\varphi_{p,q,r} = \varphi_{p,q,r}^{I}(1 + \varepsilon_{p,q,r}) \tag{32}$$

where $\varphi_{p,q,r}^{I}$ denotes the split ratio in the selected Stage I solution; $\varepsilon_{p,q,r}$ is a randomly generated perturbation in the interval $[-\delta, +\delta]$ and usually $\delta = 0.05$. On the other hand, the binary variables are adjusted one-at-a-time. Each time one z_{ij} is selected randomly. Its value is then changed from 0 to 1 or vice versa. The original MINLP model is also modified by fixing the utility levels at those in the selected initial solution. This modified model is then solved with the perturbed initial guesses to search for improved solutions. The complete solution procedure in this stage can also be found in Fig. 4.

4. Application examples

Following examples are presented to illustrate the capabilities of the modified state-space model and the effectiveness of the proposed solution strategy. Examples 1 and 2 were solved with the stage-wise superstructure by Grossmann (1991) and Yee and Grossmann (1990) respectively, while example 3 was studied by Chang and Chen (1997) with a sequential optimization approach. The proposed algorithm has been applied to identify a near global optimum in the following examples within an acceptable amount of time. A typical MINLP formulation consists of 1018–1054 constraints and 1006–1042 variables (with 32 binary variables). Using an Intel Pentium (R) D CPU 3.40 GHz computer, each GAMS run can be completed in 1.98–18.77 CPU s. To produce a satisfactory solution, about 1000 runs are usually needed in the initialization stage and another 1000 runs are executed to perturb the initial results in the second stage. Additional runs may be required to confirm the optimality conditions and to further improve the objective value. The solution quality of every case in the following subsections has been thoroughly checked by generating and comparing a large sample of solutions.

Table 1 – Stream data of example 1

Stream No. (*n*)	$F^{IN}_{1,n}$ (or $F^{OUT}_{2,n}$) (kW/K)	$T^{IN}_{1,n}$ (K)	$T^{OUT}_{2,n}$ (K)	Cost (USD kW^{-1} year^{-1})
H1	10	650	370	–
H2	20	590	370	–
C1	15	410	650	–
C2	13	353	500	–
S1	–	680	680	80
W1	–	300	320	15

$U = 0.5$ (kW m^{-2} K^{-1}) for all matches except ones involving steam. $U = 0.833$ (kW m^{-2} K^{-1}) for matches involving steam. Annualized capital cost = 5500 + 150 × (area (m^2)) for all exchangers.

4.1. *Example 1*

Let us first consider the stream data presented in Table 1 (Grossmann, 1991). In this heat-exchange system, the process hot streams H1 and H2 can be cooled by process cold streams C1 and C2. The unit costs of cold and hot utilities, i.e., W1 and S1, in this example are 15 USD kW^{-1} year^{-1} and 80 USD kW^{-1} year^{-1}, respectively. The annualized capital cost of heat exchanger is computed according to the cost model used in the original study, i.e., $5500 + 150A_{i,j}$, where the heat-transfer area $A_{i,j}$ is in m^2. Grossmann (1991) obtained an optimal network with 3 heat exchangers and 2 coolers and 1 heater, which achieved a TAC of 155,000 USD year^{-1}. The corresponding consumption rates of the cold and hot utilities are 491.15 kW and 2141.15 kW, respectively. The annualized capital investment is 83,600 USD year^{-1}.

To investigate the effects of multi-stream mixing, let us first assume that the two hot streams (i.e., H1 and H2) are allowed to be merged and the two cold streams (i.e., C1 and C2) are also mixable, while the mixing of hot and cold streams is not permitted. The state-space superstructure for this case is shown in Fig. 5. Notice that the branches of every hot stream splitter at the inlet of DN block are connected to all outlet mixers for the hot streams, while the branches of every cold stream inlet splitter are connected to all cold-stream mixers. A total of 176 different initial feasible solutions have been generated by following the proposed procedure in Stage I. These data points were classified into 3 clusters (see Fig. 6). Only one solution in the lowest cluster was selected for the refined search in the second stage. It should be noted that the darkened circles in the OP block represent the matches identified in the final optimal solution. The corresponding optimal network is also presented in Fig. 7. The minimum TAC of this network was found to be 146990.92 USD year^{-1}, which consists of an annualized capital investment of 77979.20 USD year^{-1} and a utility cost of 69011.72 USD year^{-1}. The corresponding consumption rates of the cold and hot utilities are 2148.75 kW and 459.75 kW, respectively.

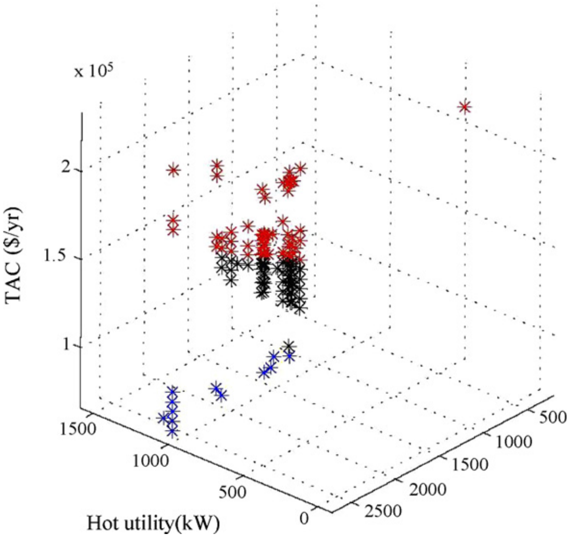

Fig. 6 – Clustering analysis.

In the second case of this example, all process streams are allowed to be mixed. A typical state-space superstructure used in our computations is provided in Fig. 8. In the DN block, every pair of splitter and mixer is connected. The resulting optimal network is presented in Fig. 9. The minimum TAC and the corresponding capital investment in this case can both be drastically reduced to 70243.33 USD year^{-1} and 16408.33 USD year^{-1}, respectively. The minimum consumption rates of the cold and hot utilities for this HEN design can also be cut down to 1989 kW and 300 kW, respectively. In addi-

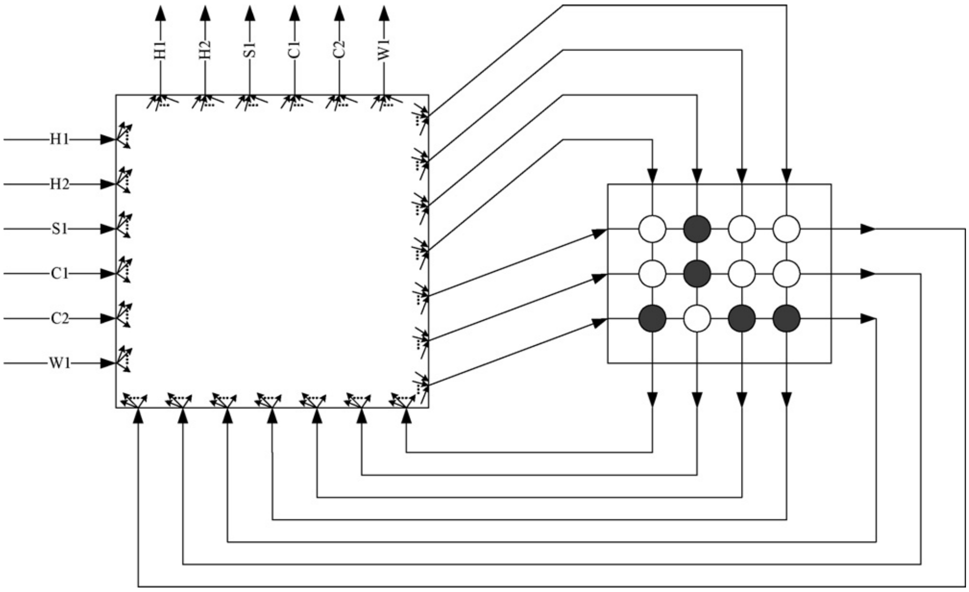

Fig. 5 – State-space superstructure used for case 1 in example 1.

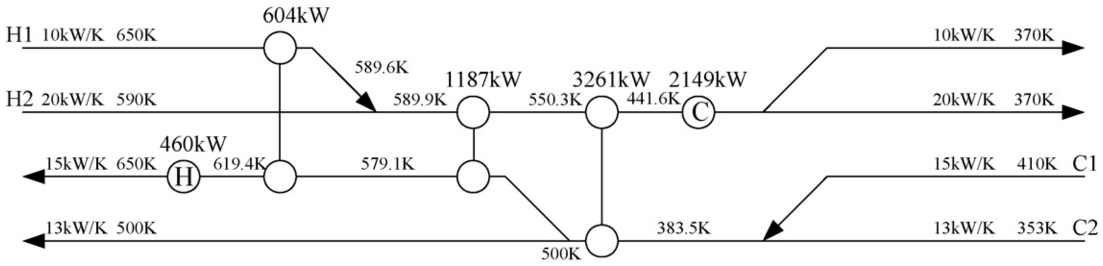

Fig. 7 – Optimal HEN design for case 1 in example 1.

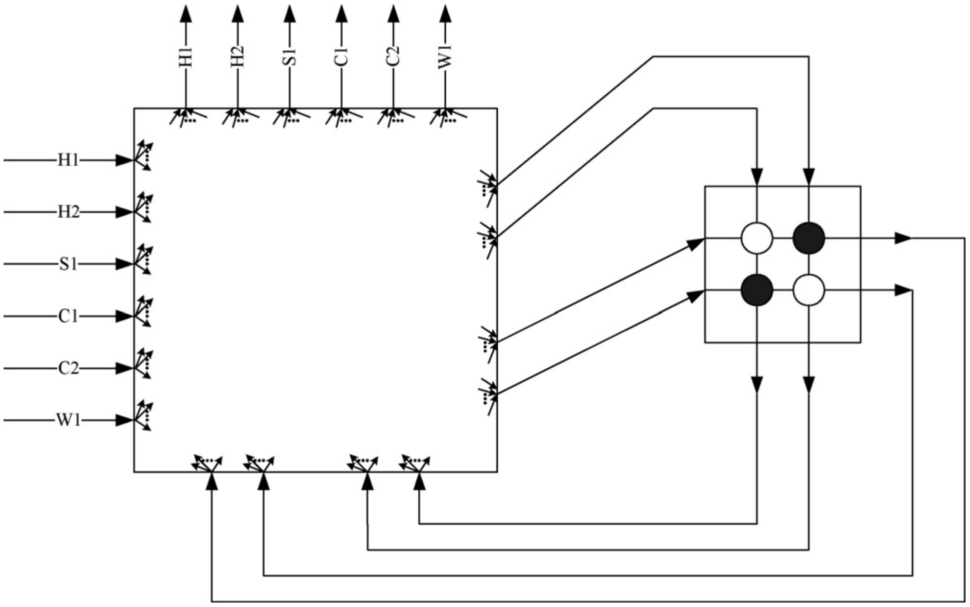

Fig. 8 – State-space superstructure used for case 2 in example 1.

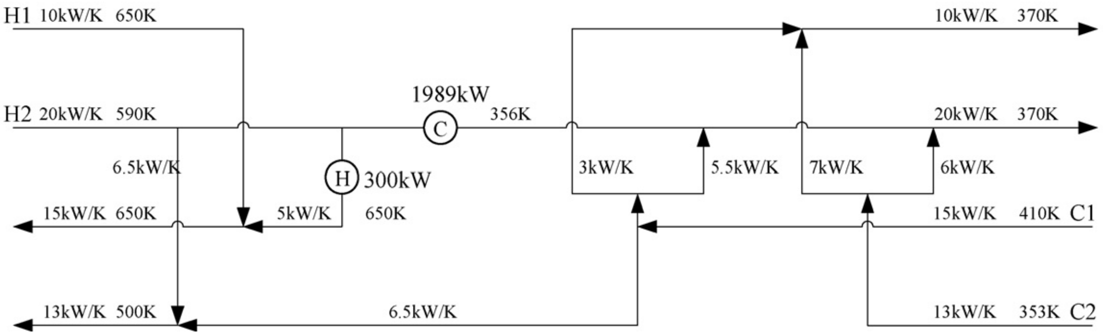

Fig. 9 – Optimal HEN design for case 2 in example 1.

tion, notice that the indirect heat exchangers are not needed in this design. Thus, it appears that both capital and operating costs can be lowered significantly if the multi-stream mixing can be considered as an added option in HEN design.

4.2. *Example 2*

Let us next consider the stream data presented in Table 2 (Yee and Grossmann, 1990). The unit costs of cold and hot utility (W1 and S1) in this example are respectively chosen to be 20 USD kW^{-1} year^{-1} and 80 USD kW^{-1} year^{-1}. The total annualized capital cost is computed with two different formulas. In particular, the cost model is $1000A_{i,j}^{0.6}$ for the indirect exchangers and $1200A_{i,j}^{0.6}$ for the heaters and coolers. The heat-transfer

Table 2 – Stream data of example 2

Stream No. (*n*)	$F^{IN}_{1,n}$ (or $F^{OUT}_{2,n}$) (kW/K)	$T^{IN}_{1,n}$ (K)	$T^{OUT}_{2,n}$ (K)	Cost (USD kW^{-1} year^{-1})
H1	30	443	333	–
H2	15	423	303	–
C1	20	293	408	–
C2	40	353	413	–
S1	–	450	450	80
W1	–	293	313	20

$U = 0.8$ (kW m^{-2} K^{-1}) for all matches except the ones involving steam. $U = 1.2$ (kW m^{-2} K^{-1}) for matches involving steam. Annualized capital cost = 1000 × (area (m^2))$^{0.6}$ for all exchangers except heaters. Annualized capital cost = 1200 × (area (m^2))$^{0.6}$ for heaters.

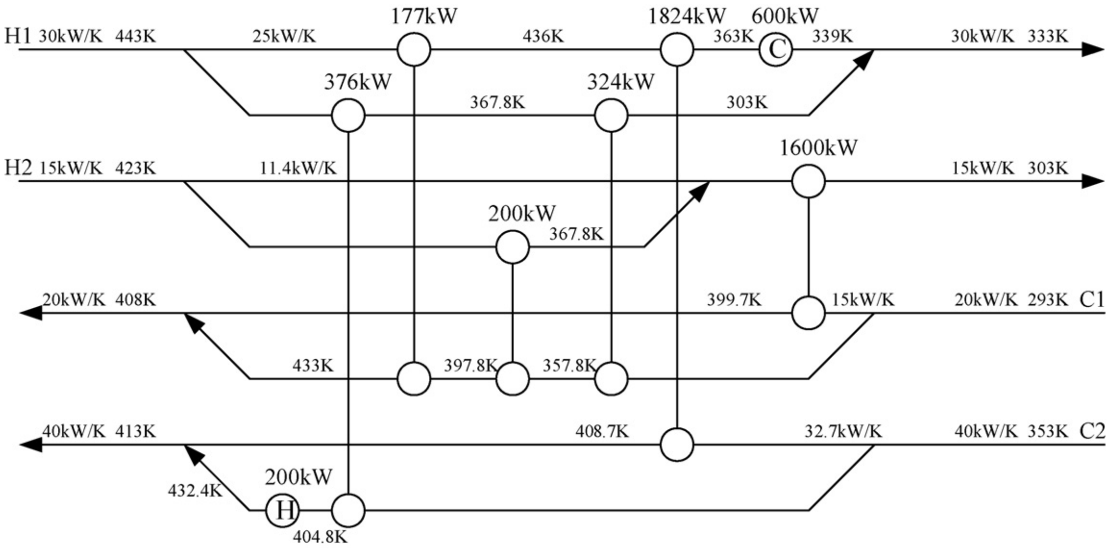

Fig. 10 – Optimal HEN design of case 1 in example 2 (using utility cost as the objective function).

area $A_{i,j}$ in these models should be again determined with the unit m^2. The optimal HEN reported by Yee and Grossmann (1990) consists of 4 exchangers, 1 cooler and 1 heater. A TAC of 89,832 USD year^{-1} (with an annualized capital investment of 61,832 USD year^{-1}) is achieved in this design. The corresponding consumption rates of the cold and hot utilities are 600 kW and 200 kW, respectively.

It is well established that, by properly selecting the objective functions, the resulting optimal HEN designs can be made to possess certain desirable feature(s). To this end, the multi-stream mixers could be used to enhance these features. Let us use two objective functions, i.e., the total utility cost and the total capital investment, to demonstrate this point. Two different cases are again adopted here. In the first case, any hot (or cold) stream is allowed to be merged with another hot (or cold) stream, while the mixing of hot and cold streams is not permitted. In case 2, all process streams are mixable.

When the utility cost is used as the objective function in case 1, the optimal network in Fig. 10 can be obtained. The minimum utility cost obtained in this solution is 28,000 USD year^{-1}, and the corresponding consumption rates of the cold and hot utilities are 600 kW and 200 kW, respectively. These results are essentially the same as those reported by Yee and Grossmann (1990). Notice that the aforementioned minimum utility levels can also be confirmed with Pinch analysis for a traditional HEN. This is not surprising since it has been shown in Chang et al. (1994) that, under the match constraints imposed in case 1, the above utility consumption rates cannot be further reduced with the multi-stream mixers. On the other hand, when the capital investment is used as the objective function, the optimal HEN in Fig. 11 can be generated. Notice that only 1 heat exchanger, 2 coolers and 1 heater are needed in this design and the minimum objective value achieved in this case is 39095.81 USD year^{-1}. This solution is significantly better in terms of capital cost than that reported the literature.

In case 2, the same solution was obtained by solving the MINLP model with either one of the two objectives functions mentioned above. The resulting optimal network structure is shown in Fig. 12. Notice that only one cooler is needed in this design. Consequently, the consumption rates of the cold and hot utilities can be reduced to 400 kW and 0 kW, respectively, and the minimum utility cost in this case, i.e., 8000 USD year^{-1}, is much lower than that predicted with Pinch method for a traditional HEN. Notice also that the minimum annualized capital cost for the HEN in Fig. 12 is 3756.36 USD year^{-1}, which represents a further (and very drastic) improvement when compared with the design in Fig. 11. In fact, the same HEN may be produced by using TAC as the objective function. This is because the design in Fig. 12 is optimal in terms of both utility and capital costs.

4.3. *Example 3*

Let us finally consider the heat-exchange system defined in Table 3, in which only process streams C2 and H2 are allowed to be mixed. The unit costs of hot utility (S1) and cold utility (W1) adopted in this example are 30 USD kW^{-1} year^{-1} and 15 USD kW^{-1} year^{-1}, respectively. The capital cost of heat exchanger is computed in this example according to $2000A_{i,j}^{0.6}$.

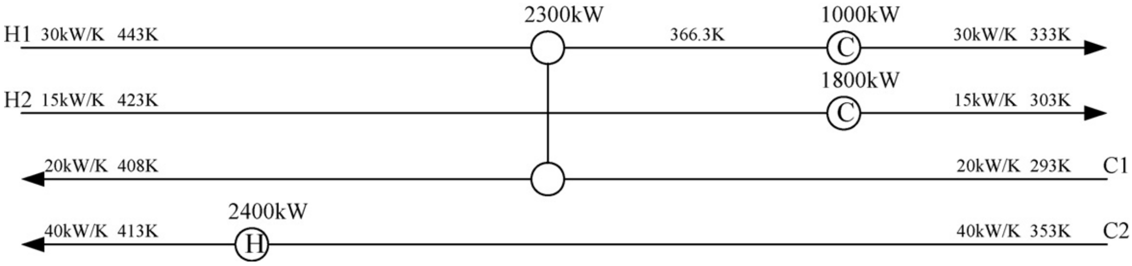

Fig. 11 – Optimal HEN design of case 1 in example 2 (using capital cost as the objective function).

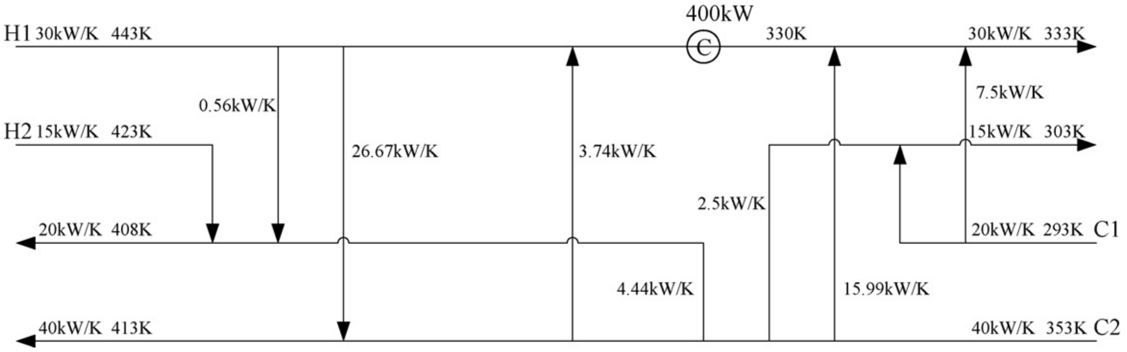

Fig. 12 – Optimal HEN design of case 2 in example 2.

This problem was originally solved by Chang and Chen (1997) with a *sequential* optimization approach according to a given minimum temperature approach of 60 °C. In this study, the minimum consumption rates of cold and hot utilities were found with a LP model to be 80 kW and 1150 kW, respectively. The corresponding optimal network structure was generated with a nonlinear program and the TAC of this HEN can be estimated to be 57891.241 USD year^{-1} according to the above-mentioned cost data.

Since it is not necessary to impose the aforementioned limitations on $\Delta T_{\min}$ in the proposed *simultaneous* optimization procedure, the resulting objective value can be further improved. By using the state-space superstructure in Fig. 13, one can then generate the optimal network structure in Fig. 14. Notice that the total annual cost is now reduced to 52939.57 USD year^{-1}. Notice also that the best minimum temperature approach in this case should be 50 °C and only hot utility is needed in this design.

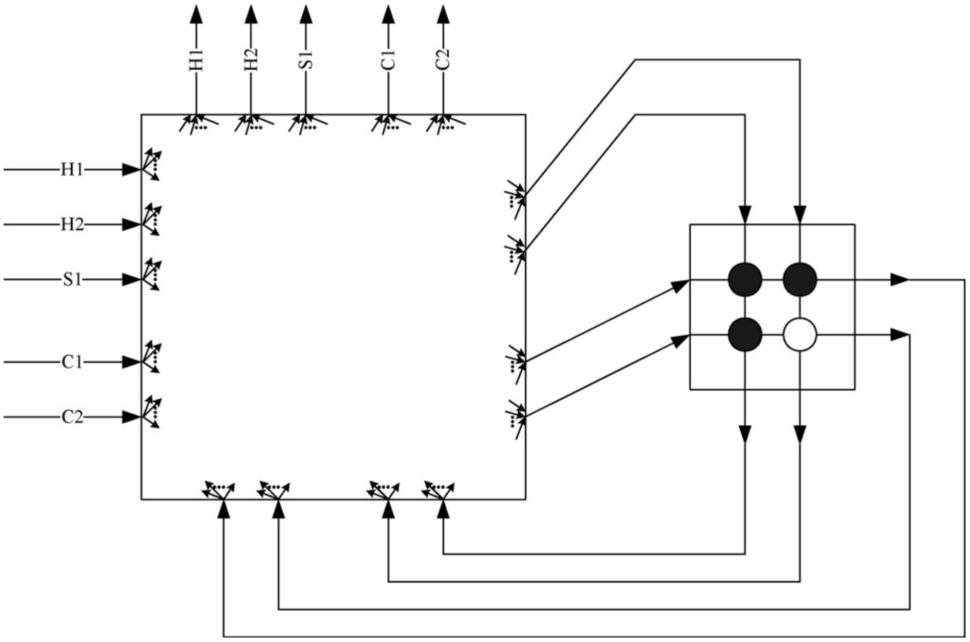

Fig. 13 – State-space superstructure used in example 3.

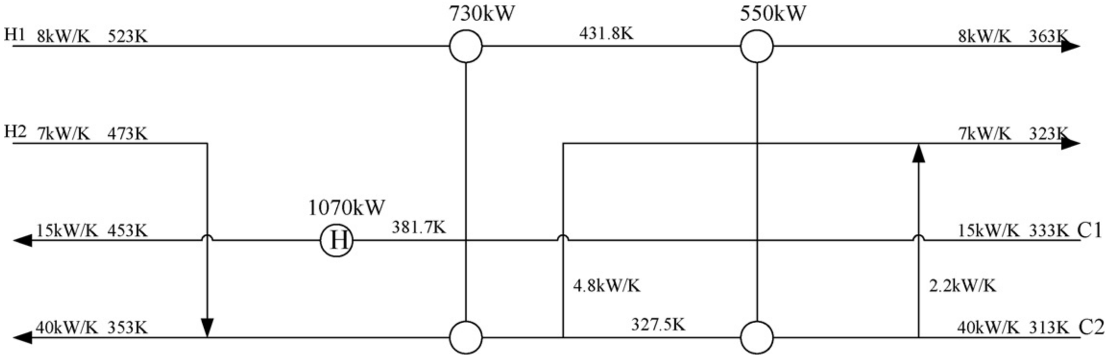

Fig. 14 – Optimal HEN design in example 3.

Table 3 – Stream data of example 3

Stream No. (n)	$F^{IN}_{1,n}$ (or $F^{OUT}_{2,n}$) (kW/K)	$T^{IN}_{1,n}$ (K)	$T^{OUT}_{2,n}$ (K)	Cost (USD kW^{-1} year^{-1})
H1	8	523	363	–
H2	7	473	323	–
C1	15	333	453	–
C2	40	313	353	–
S1	–	523	523	30
W1	–	300	300.8	15

$U = 1$ (kW m^{-2} K^{-1}) for all matches. Annualized capital cost = 2000 × (area (m^2))$^{0.6}$ for all exchangers.

5. Conclusions

The state-space superstructure has been modified in this study to formulate a MINLP model for one-step optimization of heat exchanger networks with multi-stream mixers. The advantage of this approach is that the added design options of mixing/splitting process streams can be easily incorporated in the model formulation. A two-stage search strategy has also been developed in this work to guarantee the solution quality and efficiency. In the application studies we have carried out so far, it can be clearly observed that the TACs of resulting HEN designs are indeed lower than those generated with the conventional methods. These financial savings are brought about not only by introducing additional design flexibility with mixers but also by following the proposed simultaneous optimization procedure.

Acknowledgment

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