J. Chin. Inst. Chem. Engrs., Vol. 36, No. 5, 421-432, 2005

A Novel Strategy for Synthesis of Flexible Heat-Exchange Networks

Cheng-Liang Chen[1], **Chih-Hao Kuo**[2], **and Ping-Sung Hung**[3]

Department of Chemical Engineering, National Taiwan University

Taipei 106, Taiwan

Abstract — A novel strategy for the synthesis of a cost-effective flexible heat-exchange network (HEN) that involves the expected disturbance range in the source-stream temperatures and flow rates is presented. The network synthesis problem is decomposed into four main iterative steps: (1) the synthesis of a network candidate with a minimum total annual cost (TAC); (2) flexibility analysis without consideration of the area restrictions to verify whether the current network candidate is feasible within the full, expected disturbance range; (3) integer cuts to exclude disqualified network configurations, followed by step (1) again to synthesis a new network structure; (4) with consideration of the size restriction that has been ignored previously, execution of flexibility analysis of the network qualified in step (2), with an increase of the area of individual exchange units if necessary. A few iterations of these design steps may be required to secure the desirable results. In addition to the theoretical derivation, a numerical example is provided to demonstrate the efficiency of the proposed strategy for the synthesis of a flexible heat exchange network.

Key Words : Heat exchange network (HEN), Synthesis, Flexibility, Superstructure, Mixed-integer nonlinear programming (MINLP)

INTRODUCTION

A standard heat-exchange network (HEN) synthesis problem can be stated as follows: Given hot and cold process streams to be cooled and heated, respectively, from their supplied temperatures to stated target temperatures, and given available heating and cooling utilities, synthesize a HEN configuration to reach assigned objective(s), such as the minimum utility consumption, the minimum total number of heat-exchange units, the minimum total exchanger area, the total annual cost (TAC), etc. HEN synthesis is by far one of the most developed fields. Many techniques, such as the pinch design method (Linnhoff and Hindmarsh, 1983) and mathematical programming approaches, including sequential (Floudas *et al.*, 1986) and simultaneous optimization (Yee *et al.*, 1990; Yee and Grossmann, 1990), have been proposed (Grossmann *et al.*, 1999). A thorough review of HEN synthesis methods can be found in one recent report (Furman and Sahinidis, 2002).

Such issues as minimizing the utility consumption, minimizing the matching numbers, minimizing the total area for all exchange units, and achieving flexibility in a network to enable feasible operation under possible variations in source-stream temperatures and flow rates—all typical design objectives—have also been the subjects of some articles (Marselle *et al.*, 1982; Grossmann *et al.*, 1983; Halemane and Grossmann, 1983, Swaney and Grossmann, 1985; Floudas and Grossmann, 1987; Grossmann and Floudas, 1987; Aaltola, 2002). Among them, Floudas and Grossmann (1987) proposed a sequential synthesis method that combines the multiperiod mixed-integer linear programming (MMILP) transshipment model with the active set strategy (Floudas and Grossmann, 1987) to guarantee the desired HEN flexibility. Illustrations show that a few iterations are usually required in the synthesis and flexibility analysis stages. However, the formulation and the synthesis procedure are quite tedious when it comes to the partitioning of temperature intervals under uncertain inlet temperatures. Aaltola (2002) proposed using a multiperiod simultaneous mixed-integer nonlinear programming (MINLP) model to minimize the total annual cost (TAC) and generate a flexible heat-exchange network directly. Since it does not rely on sequential decomposition, this method seems simple and straightforward. However, the operational feasibility of the resulting network is not guaranteed because only a finite number of operating conditions are examined during the design

[1] 陳誠亮, To whom all correspondence should be addressed

[2] 郭志豪

[3] 洪平松

process. Chen and Hung (2004) combined the advantages of both approaches to synthesize a flexible heat-exchange network. In their approach, however, the isothermal mixing assumption is not suitable for practical operating conditions, though this assumption can result in convex constraints.

In this paper, we extend the methodology of Chen and Hung (2004) by omitting the impractical isothermal mixing assumptions for hot/cold streams from each exchange unit, and adaptation of the unit size for exchangers is also taken into account in the flexibility analysis. In this novel approach, the flexible HEN synthesis problem is decomposed into iterative decision steps. In the simultaneous synthesis step, the problem is formulated as a mixed-integer nonlinear program (MINLP) for minimizing the TAC of the network, based on the modified stagewise superstructure proposed by Yee *et al.* (1990). The widely-adopted assumption of isothermal mixing for all hot (cold) streams is abandoned during the synthesis stage. In the flexibility analysis step, we solve the flexibility index evaluation problem for the network structure by directly applying the active set strategy (Floudas and Grossmann, 1987; Grossmann and Floudas, 1987). The restriction on the finite unit size is ignored temporarily to simplify the analysis. Should the resulting network(s) not pass the flexibility test, associated integer cuts are appended to the search space to exclude the same network(s) from further synthesis. The size of the qualified network is finally adapted to guarantee flexible operation over the whole expected disturbance range. In addition, a set of additional extreme operating points can be included to reduce the feasible space and to accelerate the design process. To obtain the final qualified network configuration, several iterations of network synthesis, flexibility analysis, and exchanger sizing are usually required. According to the results of simulations performed on one example modified from Floudas and Grossmann (1987), the efficiency of the proposed flexible HEN synthesis method is quite satisfactory.

PROPOSED STRATEGY FOR FLEXIBLE HEN SYNTHESIS

A HEN synthesis problem with N_H hot streams and N_C cold streams along with possible variations in input temperatures and heat capacity flow rates is considered here. Let $\boldsymbol{\theta}$ denote an uncertain parametric vector (e.g., input temperatures and/or flow rates) with a nominal value $\boldsymbol{\theta}^0$, $\Delta\boldsymbol{\theta}^-$, and $\Delta\boldsymbol{\theta}^+$ represent the maximum expected deviations of the uncertain parameters in the negative and positive directions. The flexible HEN synthesis problem can then be defined as that of synthesizing a cost-effective heat-exchange

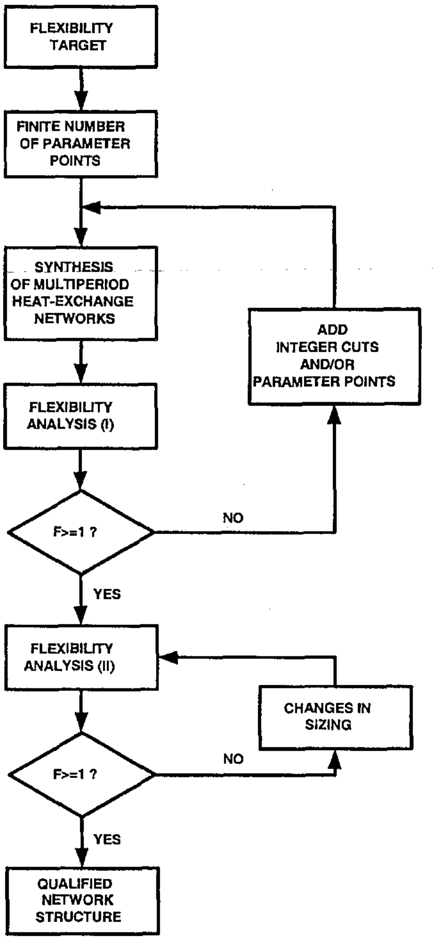

Fig. 1. Proposed strategy for flexible HEN synthesis.

network that is workable for all possible operating points contained in $P(\delta=1)$ (Floudas and Grossmann, 1987), where

$$P(\delta) = \{ \boldsymbol{\theta} \mid \boldsymbol{\theta}^0 - \delta\Delta\boldsymbol{\theta}^- \le \boldsymbol{\theta} \le \boldsymbol{\theta}^0 + \delta\Delta\boldsymbol{\theta}^+ \}. \quad (1)$$

As pointed out in the literature (Marselle *et al.*, 1982; Grossmann *et al.*, 1983; Swaney and Grossmann, 1985), this problem is difficult to solve directly because the feasible region defined by the inequality energy balance constraints is nonconvex (Floudas, 1995), so the critical point that confines the solution might not rest on the vertices of the polyhedral region of uncertainty. It is this difficulty that motivates us to divide the flexible HEN design into iterative steps, as depicted in Fig. 1. The proposed strategy for flexible HEN synthesis involves the following iterative steps:

Synthesis of a multiperiod network via simultaneous optimization

According to the modified superstructure-based multiperiod MINLP formulation for HEN synthesis discussed in next Section, a heat-exchange network can be synthesized by means of any existing mixed-

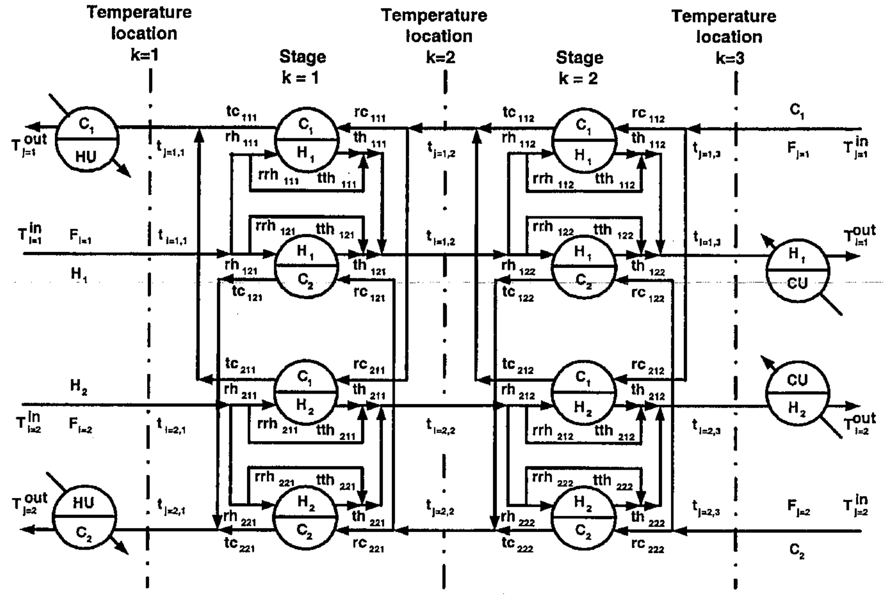

Fig. 2. The two-stage superstructure without the isothermal mixing assumption.

integer nonlinear optimization algorithm. Several extreme operating periods can be considered simultaneously to reduce the search space and to speed up the convergence, although the number of continuous variables will be increased dramatically. It should be noted that the flexibility requirement is not directly taken into account in this synthesis step in order to simplify calculation.

Evaluation of the flexibility index

Without considering the limitation imposed on the exchanger area, we evaluate the flexibility index of the network resulting from the previous synthesis step to determine whether the current network satisfies the assigned flexibility target, that is, whether the network can be operated over the full range of possible input stream temperatures and flow rates. Here, the flexibility index is determined by using the active set strategy, proposed by Grossmann and Floudas (1987) and will be reviewed lately, in order to take into account the possibility of nonextreme critical points. If the current HEN structure meets the requirement of the flexibility target, it can be temporarily accepted as a qualified network to facilitate further examination with the consideration of area constraints. On the other hand, if the resulting flexibility index does not satisfy the target, then a new network structure with improved operational flexibility must be found by using a procedure that involves the following steps.

Integer cuts to exclude disqualified networks

For disqualified network structures, the integer cuts expressed in Eq. (14) and/or some additional extreme points can be appended to the original constraints to reduce the search space, and then the synthesis step can be repeated to find a new candidate network.

Re-sizing of exchangers

For a network structure that has been qualified in the flexibility analysis step, the heat exchangers will be re-sized if necessary to guarantee flexible operation over the whole disturbance range.

Several iterations of these design steps are sometimes required to obtain a qualified configuration. Nevertheless, the proposed strategy is attractive because it avoids the need to include a large number of constraints and operating points directly in the formulation. To illustrate how the whole synthesis procedure can be performed, an example will be provided. Through numerical simulations, it can be verified that the proposed strategy is easy to implement and can provide a feasible and balanced solution for the heat-exchange network synthesis problem.

SYNTHESIS OF MULTIPERIOD HEAT-EXCHANGE NETWORKS

The stagewise superstructure proposed by Yee and Grossmann (1990) is adopted and is modified to construct the configuration of a heat-exchange network, as it is suitable for formulating a simultaneous solution that considers the total utility consumption, the total number of matches, and the total area of the heat-exchange units. A two-stage superstructure with two hot and two cold streams is illustrated in Fig. 2

for reference; the definitions of relevant notations for the structure can be found in the Nomenclature. It should be noted that by-passing of a hot stream around each exchange unit is allowable and non-isothermal mixing of hot/cold streams is also admitted in the proposed superstructure.

Instead of directly considering all possible combinations of uncertain input temperatures and heat capacity flow rates for flexible network synthesis, we only take into account a finite number of extreme operating conditions to reduce the search space. The mathematical programming formulation for minimizing the total annual cost, TAC, which includes the average costs of both hot and cold utility consumption over a finite number of operating points and the annualized costs of the installation and materials of the heat-exchange units, can be summarized as follows (Yee *et al.*, 1990; Yee and Grossmann, 1990; Biegler *et al.*,1997; Chen and Hung, 2004):

$$\min_{\mathbf{x}\in\Omega} TAC = \frac{1}{N_V+1}\Big(\sum_{\forall n\in VT}\sum_{\forall i\in HP} C_{cu}\,qcu_i^{(n)} + \sum_{\forall n\in VT}\sum_{\forall j\in CP} C_{hu}\,qhu_j^{(n)}\Big)$$
$$+ \sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST} C_{ij}\Big[\max_{\forall n\in VT}\Big(\frac{q_{ijk}^{(n)}}{U_{ij}LMTD_{ijk}^{(n)}}\Big)\Big]^{\beta_{ij}}$$
$$+ \sum_{\forall j\in CP} C_{ij}\Big[\max_{\forall n\in VT}\Big(\frac{qhu_j^{(n)}}{U_{hu,j}LMTD_{hu,j}^{(n)}}\Big)\Big]^{\beta_{i,cu}}$$
$$+ \sum_{\forall i\in HP} C_{i,cu}\Big[\max_{\forall n\in VT}\Big(\frac{qcu_i^{(n)}}{U_{i,cu}LMTD_{i,cu}^{(n)}}\Big)\Big]^{\beta_{hu,j}}, \qquad (2)$$

where $VT = \{0, 1, \ldots, N_V\}$ is the index set, in which zero denotes the nominal conditions (or the base case) for numbering a limited number of extreme operating conditions used to find the optimal final structure. These possible operating vertices are applied here to reduce the search space. $\mathbf{x}$ and $\mathbf{\Omega}$ denote the vector of design variables and the feasible search space comprising all material/energy balance constraints and relevant logical constraints, respectively:

$$\mathbf{x} \equiv \left\{\begin{array}{r} t_{ik}^{(n)}, t_{jk}^{(n)}, t_{i,N_T+1}^{(n)}, t_{j,N_T+1}^{(n)}, th_{ijk}^{(n)}, tc_{ijk}^{(n)}, tth_{ijk}^{(n)}; \\ rh_{ijk}^{(n)}, rc_{ijk}^{(n)}, rrh_{ijk}^{(n)}, q_{ijk}^{(n)}, q_{i,cu}^{(n)}, q_{hu,j}^{(n)}; \\ dth_{ijk}^{(n)}, dtc_{ijk}^{(n)}, dt_{i,cu}^{(n)}, dt_{hu,j}^{(n)}; \\ z_{ijk}, z_{i,cu}, z_{hu,j} \\ \forall_i \in HP, j\in CP, k\in ST, n\in VT \end{array}\right\} \qquad (3)$$

$$\mathbf{\Omega} = \left\{ \mathbf{x} \;\middle|\; \begin{array}{ll}
\left.\begin{array}{r} (T_i^{in(n)} - T_i^{out})F_i^{(n)} = \sum_{\forall k\in ST}\sum_{\forall j\in CP} q_{ijk}^{(n)} + qcu_i^{(n)} \\ (T_j^{out} - T_j^{in(n)})F_j^{(n)} = \sum_{\forall k\in ST}\sum_{\forall i\in HP} q_{ijk}^{(n)} + qhu_j^{(n)} \end{array}\right\} & \text{overall heat balances} \\
\left.\begin{array}{r} (t_{ik}^{(n)} - t_{i,k+1}^{(n)})F_i^{(n)} = \sum_{\forall j\in CP} q_{ijk}^{(n)} \\ (t_{jk}^{(n)} - t_{j,k+1}^{(n)})F_j^{(n)} = \sum_{\forall i\in HP} q_{ijk}^{(n)} \end{array}\right\} & \text{stage-wise heat balances} \\
\left.\begin{array}{l} rh_{ijk}^{(n)}F_i^{(n)}(t_{ik}^{(n)} - th_{ijk}^{(n)}) = q_{ijk}^{(n)} \\ rc_{ijk}^{(n)}F_j^{(n)}(tc_{ijk}^{(n)} - t_{j,k+1}^{(n)}) = q_{ijk}^{(n)} \\ rh_{ijk}^{(n)}F_i^{(n)}(1 - rrh_{ijk}^{(n)})(t_{ik}^{(n)} - tth_{ijk}^{(n)}) = q_{ijk}^{(n)} \end{array}\right\} & \text{heat balances for each exchanger} \\
\left.\sum_{\forall j\in CP} rh_{ijk}^{(n)} = 1,\ \sum_{\forall i\in HP} rc_{ijk}^{(n)} = 1 \right\} & \text{sum of split ratios} \\
\left. t_{i1}^{(n)} = T_i^{in(n)},\ t_{j,N_T+1}^{(n)} = T_j^{in(n)} \right\} & \text{assignment of inlet temp.} \\
\left.\begin{array}{r} t_{ik}^{(n)} \ge t_{i,k+1}^{(n)}, \quad t_{jk}^{(n)} \ge t_{j,k+1}^{(n)} \\ T_i^{out} \le t_{i,N_T+1}^{(n)}, T_j^{out} \ge t_{j1}^{(n)} \end{array}\right\} & \text{feasibility of temperatures} \\
\left.\begin{array}{r} (t_{i,N_T+1}^{(n)} - T_i^{out(n)})F_i = qcu_i^{(n)} \\ (T_j^{out(n)} - t_{j1}^{(n)})F_j^{(n)} = qhu_j^{(n)} \end{array}\right\} & \text{utility loads} \\
\left.\begin{array}{r} q_{ijk}^{(n)} - \Lambda_{ij}z_{ijk} \le 0 \\ qcu_i^{(n)} - \Lambda_i zcu_i \le 0 \\ qhu_j^{(n)} - \Lambda_j zhu_j \le 0 \end{array}\right\} & \text{heat loads constraints} \\
\left.\begin{array}{l} dth_{kjk}^{(n)} \le t_{ik}^{(n)} - tc_{ijk}^{(n)} + \Gamma_{ij}(1 - z_{ijk}) \\ dtc_{kjk}^{(n)} \le tth_{ijk}^{(n)} - t_{j,k+1}^{(n)} + \Gamma_{ij}(1 - z_{ijk}) \\ dtcu_j^{(n)} \le t_{i,N_T+1}^{(n)} - T_{cu}^{out} + \Gamma_i(1 - zcu_i) \\ dthu_j^{(n)} \le T_{hu}^{out} - t_{j1}^{(n)} + \Gamma_j(1 - zhu_j) \end{array}\right\} & \text{approach temperatures} \\
\left. dth_{ijk}^{(n)}, dtc_{ijk}^{(n)}, dtcu_i^{(n)}, dthu_i^{(n)} \ge \Delta T_{\min} \right\} & \text{approach temp. bounds} \\
\left.\begin{array}{l} t_{ik}^{(n)}, t_{jk}^{(n)}, t_{i,N_T+1}^{(n)}, t_{j,N_T+1}^{(n)}, th_{ijk}^{(n)}, tc_{ijk}^{(n)}, tth_{ijk}^{(n)}, \\ rh_{ijk}^{(n)}, rc_{ijk}^{(n)}, rrh_{ijk}^{(n)}, q_{ijk}^{(n)}, qi_{i,cu}^{(n)}, q_{hu,j}^{(n)}, \\ dth_{ijk}^{(n)}, dtc_{ijk}^{(n)}, dt_{i,cu}^{(n)}, dt_{hu,j}^{(n)} \ge 0 \end{array}\right\} & \text{design variables}
\end{array} \right\} \qquad (4)$$

Here, $LMTD_{ijk}$ is the log-mean approaching temperature for matching hot stream i and cold stream j at the kth stage. Notably, the widely-adopted but impractical assumption of isothermal mixing of all hot/cold streams is abandoned, as highlighted in Eq. (4), in order to allow for a more general situation. The split ratio of a hot stream by-passing a unit is also a design variable in this model. Chen's approximation is used for $LMTD_{ijk}$ (Chen, 1987). $LMTD_{i,cu}$ and $LMTD_{hu,j}$ are defined and approximated similarly:

$$LMTD_{ijk} = \frac{dth_{ijk} - dtc_{ijk}}{\ln\dfrac{dth_{ijk}}{dtc_{ijk}}} \cong \Big[dth_{ijk}dtc_{ijk}\Big(\frac{dth_{ijk} + dtc_{ijk}}{2}\Big)\Big]^{1/3}. \qquad (5)$$

Noted that the inclusion of each of the extreme periods will increase the total number of continuous variables; therefore, the designer should make a trade-off between the number of variables and the searching space. There are total $4^{N_H+N_C}$ vertices for a HEN synthesis problem with N_H hot and N_C cold streams that may vary in temperatures and flow rates. It is impractical to include simultaneously all those operating extremes for resilient network design due to the dramatic increase of the number of continuous variables for each of these excessive situations. Marselle *et al.* (1982) suggest considering those statuses that tend to maximize the need for exchangers, coolers, and heaters, as are showed as follows. The case of all streams with the maximum heat capacity flow rates and with the maximum (minimum) supply temperatures for all hot (cold) streams tends to result in a network configuration with the maximum heat exchange area. The instance of the highest cooling requirement (*i.e.*, all hot streams have the upper bound temperatures and heat capacity flow rates) and the lowest cooling capability (all cold streams have the upper bound temperatures and the lower bound heat capacity flow rates) inclines to be a network consuming the maximum cooling utility. A network needs the maximum heating utility should the highest heating requirement for the cold streams (minimum temperatures and maximum flow rates) companion the lowest heating capability for hot streams (minimum temperatures and flow rates). As pointed out by Marselle *et al.* (1982), a network that can handle these three extreme periods does not necessarily imply that all states within the disturbance range can be operated adequately. Although a quantitative flexibility analysis is still relevant to clarify the feasible operating range of the network, the network combining these three extreme periods represents a good resilient network candidate. Other vertices are seldom applied for design in the literature except for those problems considering uncertain supply temperatures only (Konukman *et al.*, 2002).

FLEXIBILITY ANALYSIS

The solution of Eq. (2) is a heat-exchange network with a minimum *TAC* under a specific configuration that satisfies multiple extreme operating conditions. When the resulting network is applied to a process where the source-stream temperatures and heat capacity flow rates can vary over the full range of expected variation, its flexibility can be measured by means of the flexibility index defined by Swaney and Grossmann (1985). To carry out flexibility analysis, all relevant equality and inequality constraints for the heat-exchange network model, except for the area constraints, can be reorganized as described in Eqs. (6)-(7):

$$\mathbf{h}(\mathbf{d},\mathbf{u},\mathbf{w},\boldsymbol{\theta}) = \begin{Bmatrix} q_{ijk} - rh_{ijk}F_i(t_{ik} - th_{ijk}) \\ q_{ijk} - rc_{ijk}F_j(tc_{ijk} - t_{j,k+1}) \\ qcu_i - F_i(t_{i,N_T+1} - T_i^{out}) \\ qhu_j - F_j(T_j^{out} - t_{j1}) \\ \sum_{j\in J} rh_{ijk} - 1 \\ \sum_{i\in I} rc_{ijk} - 1 \\ T_i^{in} - t_{i1} \\ T_j^{in} - t_{j,N_T+1} \end{Bmatrix} = 0, \quad (6)$$

$$\mathbf{g}(\mathbf{d},\mathbf{u},\mathbf{w},\boldsymbol{\theta}) = \begin{Bmatrix} \Delta T_{min} + t_{jk} - t_{ik} \\ \Delta T_{min} + t_{j,N_{T+1}} - t_{i,N_{T+1}} \\ \Delta T_{min} + T_{CU}^{out} - t_{i,N_{T+1}} \\ \Delta T_{min} + t_{j,1} - T_{HU}^{out} \\ -q_{ijk} \\ -F_i \\ -F_j \end{Bmatrix} \le 0. \quad (7)$$

The variables in these equations are classified into four categories. $\boldsymbol{\theta}$ is the vector of uncertain parameters (*i.e.*, temperatures and flow rates defined in Eq. (1)). The design variables **d**, obtained from the synthesis step, define the network structure and the sizes of the heat-exchange units. The control variables **u** represent the degrees of freedom in the operation of the network. **w**, the state variables, can be expressed as implicit functions of the control variables **u** and uncertain parameters $\boldsymbol{\theta}$ by solving the independent equality constraints:

$$\mathbf{h}(\mathbf{d},\mathbf{u},\mathbf{w},\boldsymbol{\theta}) = 0 \Rightarrow \mathbf{w} = \mathbf{w}(\mathbf{d},\mathbf{u},\boldsymbol{\theta}). \quad (8)$$

Thus, the inequalities of the network can be represented by the following equation, where CI is the index set of condensed inequalities:

$$g_m[\mathbf{d},\mathbf{u},\mathbf{w}(\mathbf{d},\mathbf{u},\boldsymbol{\theta}),\boldsymbol{\theta}] = f_m(\mathbf{d},\mathbf{u},\boldsymbol{\theta}) \le 0 \quad \forall m \in CI \quad (9)$$

By rearranging the related equations, we can formulate the flexibility index problem of a network as the following mixed-integer nonlinear programming problem (Grossmann and Floudas, 1987; Floudas and Grossmann, 1987; Biegler *et al.*, 1997):

$$F = \min_{\boldsymbol{\theta},\mathbf{u},s_m,\lambda_m,y_m,\delta} \delta,$$

$$\text{s.t.} \; s_m + f_m(\mathbf{d},\mathbf{u},\boldsymbol{\theta}) = 0$$

$$\left.\begin{matrix} \sum_{\forall m\in CI} \lambda_m \dfrac{\partial f_m}{\partial \mathbf{u}} = 0, \\ \sum_{\forall m\in CI} \lambda_m = 1 \\ \lambda_m - y_m \le 0 \end{matrix}\right\}*,$$

$$s_m - V(1-y_m) \le 0$$
$$\sum_{\forall m \in CI} y_m = n_u + 1,$$
$$\boldsymbol{\theta} \in P(\delta);\; y_m \in \{0,1\},$$
$$\delta, \lambda_m, s_m \ge 0,\; \forall m \in CI. \qquad (10)$$

In these equations, F represents the level of flexibility, where an F value less than 1 means that the network is not operable within the full range of definite uncertain parametric bounds; s_m are slack variables; λ_m are Kuhn-Tucker multipliers; $y_m = 1$ indicates active constraints; V is a sufficiently large real number; and n_u is the number of control variables **u**. Details of the above MINLP formulation can be found in the literature (Grossmann and Floudas, 1987; Floudas and Grossmann, 1987).

The active set strategy, as illustrated in Eq. (10), for solving the mixed-integer optimization problem consists of three basic steps (Grossmann and Floudas, 1987; Floudas and Grossmann, 1987). First, the active candidate sets should be identified. Let $N_{AS} = \{1, \ldots, n_{AS}\}$ denote the index set of all possible combinations for the active constraints, and let $AS(k)$ represent the k^{th} index set of the active constraints. Then, a value of δ^k for the kth active candidate set can be obtained by solving the following nonlinear programming (NLP) problem (Floudas and Grossmann, 1987):

$$\delta^k = \min_{\boldsymbol{\theta},\mathbf{u},\delta} \delta,$$
$$\text{s.t.}\quad f_m(\mathbf{d},\mathbf{u},\boldsymbol{\theta}) = 0,$$
$$\boldsymbol{\theta} \in P(\delta),$$
$$\delta \ge 0,$$
$$\forall m \in AS(k) \subseteq CI \qquad (11)$$

The solution of the flexibility index problem is given by

$$F = \min_{\forall k \in N_{AS}} \delta^k. \qquad (12)$$

Notice that for a problem in which there is no control variable (*i.e.*, $n_u = 0$), the flexibility analysis problem is much simpler (Grossmann and Floudas, 1987). In such a case, the stationary conditions in Eq. (10), that is, the three relations marked with a $*$ and the associated Kuhn-Tucker multipliers, λ_m, can be eliminated. In this condensed formulation, only one constraint is allowed to be active for each active set. Eq. (10) can, thus, be decomposed in terms of each individual constraint, that is, $AS(k) = \{k\}, \forall k \in N_{AS}$. The flexibility index problem, therefore, becomes significantly simpler. It should be noted that the nonlinear constraint, $q_{ijk} - U_{ij}A_{ijk}(LMTD_{ijk}) \le 0$, is included only when the re-sizing problem of a network is to be solved.

INTEGER CUTS FOR EXCLUDING THE DISQUALIFIED NETWORKS

If a heat-exchange network resulting from the previous formulation is not qualified by the flexibility test, a different network structure should be provided as a new candidate. To avoid obtaining a HEN structure that has been eliminated in the previous n_R iterations, one can add some constraints to the $(n_R+1)^{\text{th}}$ synthesis formulation. Two kinds of networks are guaranteed to be new (Chen and Hung, 2004): one type has at least one unit that is different from those in any earlier eliminated network, and the other has units that are only the same as some units in any earlier eliminated network. These two conditions can be expressed by the following logic constraints for the $(n_R+1)^{\text{th}}$ network:

$$\sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}(1-z_{ijk}^{l})z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}(1-z_{i,cu}^{l})z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}(1-z_{hu,j}^{l})z_{hu,j}^{n_R+1} \ge 1$$
$$\text{and}\quad \sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}z_{ijk}^{l}z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}z_{i,cu}^{l}z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}z_{hu,j}^{l}z_{hu,j}^{n_R+1} \le n_{SN}^{l} \;\text{(Case 1)},$$
$$\sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}(1-z_{ijk}^{l})z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}(1-z_{i,cu}^{l})z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}(1-z_{hu,j}^{l})z_{hu,j}^{n_R+1} \ge 0$$
$$\text{and}\quad \sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}z_{ijk}^{l}z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}z_{i,cu}^{l}z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}z_{hu,j}^{l}z_{hu,j}^{n_R+1} < n_{SN}^{l} \;\text{(Case 2)},$$
$$\forall l = 1,\ldots,n_R. \qquad (13)$$

These two cases can be expressed as a single integer cut equation (Chen and Hung, 2004). The integer cuts in the search space can guarantee that a network candidate that is different from all previously disqualified configurations can be obtained:

$$2\{\sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}z_{ijk}^{l}z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}z_{i,cu}^{l}z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}z_{hu,j}^{l}z_{hu,j}^{n_R+1}\}$$
$$-\{\sum_{\forall i\in HP}\sum_{\forall j\in CP}\sum_{\forall k\in ST}z_{ijk}^{n_R+1} + \sum_{\forall i\in HP}z_{i,cu}^{n_R+1} + \sum_{\forall j\in CP}z_{hu,j}^{n_R+1}\} \le n_{SN}^{l} - 1,$$
$$l = 1, \ldots, n_R. \qquad (14)$$

Table 1. Cost data for the example.

Steam cost	171.428×10^{-4} \$/kWh
Cooling water cost	60.576×10^{-4} \$/kWh
Operating time	8,600 h/yr
Exchanger capital cost	$4{,}333A^{0.6}$ A = exchanger area (m^2)
Capital annual factor	0.2

Table 2. Nominal and multi-period operating conditions for the example.

Process Streams	Heat-Capacity Flow Rate FCp (kW/K)	Input Temperature T^{in} (K)	Output Temperature T^{out} (K)
	nominal conditions (base case)		
hot stream 1 (H1)	1.4	583	323
hot stream 2 (H2)	2.0	723	553
cold stream 1 (C1)	3.0	313	393
cold stream 2 (C2)	2.0	388	553
hot utility (HU)	–	573	573
cold utility (CU)	–	303	323
	period 1 (maximum total heat-exchange load)		
hot stream 1 (H1)	1.8	593	323
hot stream 2 (H2)	2.0	723	553
cold stream 1 (C1)	3.0	313	393
cold stream 2 (C2)	2.4	383	553
	period 2 (maximum cooling load)		
hot stream 1 (H1)	1.8	593	323
hot stream 2 (H2)	2.0	723	553
cold stream 1 (C1)	3.0	313	393
cold stream 2 (C2)	1.6	393	553
	period 3 (maximum heating load)		
hot stream 1 (H1)	1.0	573	323
hot stream 2 (H2)	2.0	723	553
cold stream 1 (C1)	3.0	313	393
cold stream 2 (C2)	2.4	383	553

Note: ΔT_{min} = 10 K; U = 0.08 (kW·m^{-2}·K^{-1}) for all matches.

NUMERICAL EXAMPLE

One example with two hot/two cold streams, adapted from Floudas and Grossmann (1987), will be used here to demonstrate the efficiency of the proposed strategy. To solve the MINLP for the HENS model, the General Algebraic Modeling System GAMS (Brooke et al., 1998) is used as the main solution tool. The MINLP solver is SBB, which is based on a combination of the standard Branch and Bound (B&B) method known from Mixed Integer Linear Programming, and the NLP solver is CONOPT3 in the example.

This example involves two hot and two cold streams ($N_H = 2, N_C = 2$) along with steam and cooling water, respectively, as the heating and cooling utilities. The data for the problem, including the nominal operating conditions and three periods of extreme operating conditions, are listed in Tables 1 and 2. Suppose the expected maximum operating disturbances are ±10 K for hot stream 1 and ±5 K for cold stream 2 for the temperature and $\pm$ 0.4 kW$\cdot$K^{-1} for both hot stream 1 and cold stream 2 for the heat capacity flow rate; the objective is to derive a heat-exchange network configuration that is feasible for the given disturbance range and features the minimum TAC. The minimum number of stages in the superstructure, N_T, is set to be 2 because $\max\{N_H, N_C\} = 2$ (Yee *et al.*, 1990). The proposed iterative solution strategy is illustrated in the following. To show the effects of appending the extreme operating periods mentioned previously and of the integer cuts on the reduction of the search space, one extreme period and one integer cut per iteration are added to the model until a feasible solution is achieved. Also noted that several initials should be tried to guarantee the robustness of the final results, since we apply some local optimization solvers.

Iteration 1

To start, by applying the nominal conditions

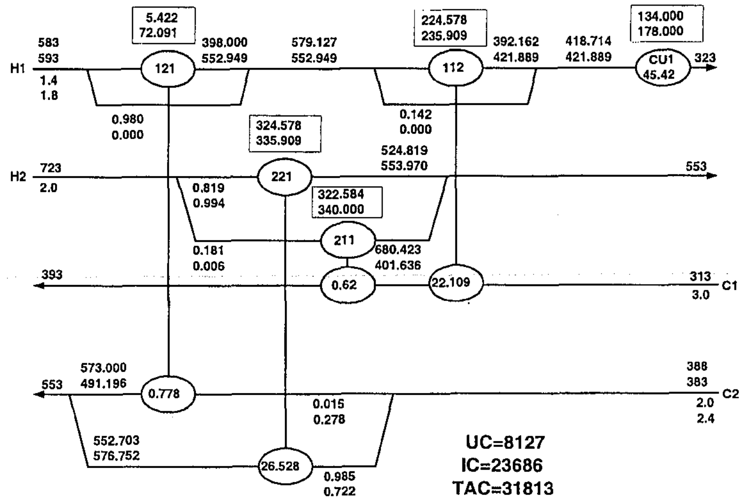

Fig. 3. HEN structure for the example with consideration of the nominal conditions and period 1 for synthesis.

Table 3. Comparison of the annual capital cost, the operating cost, and the total annual cost of the resulting networks for the example.

		Annual Capital Cost ($/yr) (investment cost, IC)	Operating Cost ($) (utility cost, UC)	Total Annual Cost ($) (TAC)
Nominal & period 1	non-isothermal	23,686	8,127	31,813
	isothermal	27,092	8,127	35,219
Nominal & period 1 ~ 2	non-isothermal	25,762	11,148	36,910
	isothermal	26,125	11,149	37,274
Nominal & period 1 ~ 3	non-isothermal	28,913	11,907	40,820
	isothermal	30,104	11,772	41,876
Sequential	non-isothermal	39,380	10,499	49,879

and period 1 to Eqs. (2)-(4), we can obtain a network with a minimum TAC of $31, 813/year, and its structure and the data for the flow rate and temperature are shown in Fig. 3, where the heat-exchange load for each unit is enclosed in a box. Let $SN^1 = \{z^1_{112}, z^1_{121}, z^1_{211}, z^1_{221}, zcu^1_1\}$ denote the set of selected units of the first candidate network. The constraints Eq. (6) and Eq. (7) are then utilized to examine this network. Because there are three control variables, there are four active constraints. These constraints can also be found in Chen and Hung (2004). Solving the nonlinear programming problem, Eq. (11), for each active set of constraints results in a flexibility index value of F = 0.6358. Such a low value of the flexibility index implies that the network structure designed for the base case will be infeasible for some possible input conditions within the disturbance range. Thus, to obtain a better network, an additional parameter point that embraces the the maximum total heat-exchange load (*i.e.*, $F^U_{H1}, F^U_{C2}, T^U_{H1}, T^L_{C2}$) and the integer cut, Eq. (14), with SN^1 and n^1_{SN} = 5 to exclude the current network configuration is appended to the network synthesis problem.

Iteration 2

With the integer cut for excluding the current network obtained in iteration 1, Eqs. (2)-(4) are solved again by simultaneously considering the conditions of periods 1 and 2 as well as the nominal operating case. The resulting network, shown in Fig. 4, features a slightly higher *TAC* value of $36,910/yr, with the set of selected units $SN^2 = \{z^2_{112}, z^2_{121}, z^2_{221}, zcu^2_1, zcu^2_2\}$ and $n^2_{SN} = 5$. The inequalities in Eqs. (6) and (7) for computing flexibility are then employed to test the operation feasibility of this network structure under the assigned operating range. Because there are two control variables, there are three active constraints. The solution of the nonlinear programming problem, Eq. (11), again shows that F = 0.6358; therefore, this network is also disqualified. Once again, a new parameter point that incorporates the maximum cooling load (*i.e.*, $F^U_{H1}, F^L_{C2}, T^U_{H1}, T^U_{C2}$) and the integer cuts to rule out the networks obtained in the first and the second iterations is introduced into the constraint set. This is followed by the third iteration.

Iteration 3

From the same Eqs. (2)-(4) and with application of the nominal operating conditions, three periods and the integer cuts for excluding the networks obtained in iterations 1 and 2, a new configuration is

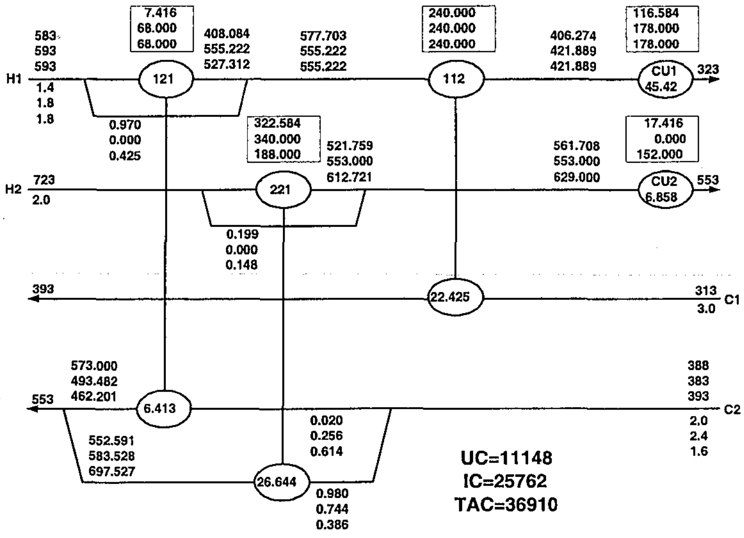

Fig. 4. HEN structure for the example with consideration of the nominal conditions and periods 1~2 for synthesis.

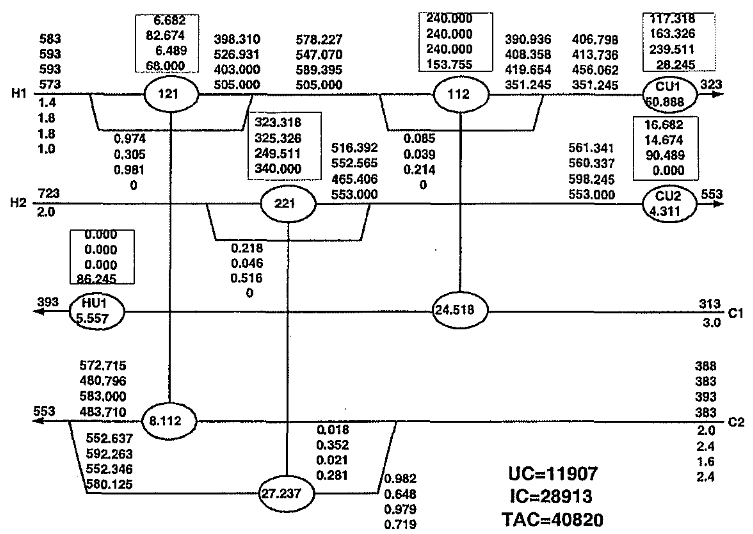

Fig. 5. HEN structure for the example with consideration of the nominal conditions and periods 1~3 for synthesis.

generated as shown in Fig. 5. It features a *TAC* of \$40,820/year, and the set of selected units $SN^3 = \{ z^3_{112}, z^3_{121}, z^3_{221}, zcu^3_1, zcu^3_2, zhu^3_1 \}$ with $n^3_{SN} = 6$. Note that one additional heater is added because of the inclusion of maximization of the heating load (*i.e.*, $F^L_{H1}, F^U_{C2}, T^L_{H1}, T^L_{C2}$). To test the operational feasibility of this network, we employ three control variables. A flexibility index value of F = 1.7134 is found by solving the nonlinear programming problem, Eq. (11), for each possible active set of constraints. Therefore, we include the area constraint, $q_{ijk} - U_{ij} A_{ijk} (LMTD_{ijk}) \le 0$, in Eq. (11). When the area of the exchangers is not expanded, the flexibility index becomes F = 1.084. This value indicates that the network structure derived in the third synthesis step is not only economical, but also feasible for the overall operating space, and this terminates the whole search process. The annualized capital cost (the investment cost, IC), the operating cost (the utility cost, UC), and the total annual cost of the resulting networks for the example are reported in Table 3 for the purpose of comparison. Also, the network structures and operating costs between nonisothermal and isothermal mixing are almost the same, and non-isothermal mixing with less annual capital costs than isothermal.

CONCLUSION

In this paper, a new strategy for synthesizing flexible heat-exchange networks that involve uncertain source-stream temperatures and flow rates has been proposed. The design problem is decomposed into iterative steps: First, the MINLP formulation is applied for the synthesis of a network configuration that bears the minimum total annual cost, with consideration of a finite number of extreme operating points that tend to maximize the need for heat exchangers, coolers, and heaters. The non-isothermal mixing of hot/cold streams for each heat-exchange unit is allowed in the formulation. Second, the active set strategy is employed in flexibility analysis to test the operational feasibility of the resulting network over the full range of expected variation of the source-stream temperatures and flow rates. The area constraints are not considered, however, in order to simplify the analysis. If the network structure does not satisfy the assigned flexibility target, then the current network is excluded by appending some integer cuts to the feasible network constraint set, and then the search process reverts to the synthesis step to find a new candidate network. If the network passes the simplified flexibility test, then the areas of the exchangers are taken into account and the flexibility index problem is solved again by including the area constraints. One can make changes only in the sizes of the heat exchangers in order to obtain a network that is feasible over the whole expected disturbance range. Sometimes, several iterations are required to obtain the final qualified network. By means of a numerical example, we have demonstrated that the proposed new strategy can generate a feasible heat-exchange network for uncertain supply temperatures and flow rates in a relatively efficient way.

ACKNOWLEDGEMENT

This work was supported by the National Science Council (R.O.C.) under contract NSC 91-ET-7-002-004-ET. Partial financial support from the Ministry of Economic Affairs under grant 92-EC-17-A-09-S1-019 is gratefully acknowledged.

NOMENCLATURE

Indices

i	hot process stream
j	cold process stream
k	superstructure stage
n	multiperiods limiting the operating conditions

Sets

$AS(k)$	the kth index set of active constraints
CI	the index set of condensed inequalities
CP	cold process stream
HP	hot process stream
N_{AS}	all possible combinations of active constraints
SN	selected units
ST	superstructure stages
VT	multiperiod operating conditions (base case included)

Parameters

F	heat capacity flow rate
N_C	number of cold streams
N_H	number of hot streams
N_T	number of superstructure stages
N_V	number of operating conditions considered for multiperiod-based design
T^{in}	inlet temperature of stream
T^{out}	outlet temperature of stream
U	overall heat-transfer coefficient
V	upper bound on slack variables
Λ	upper bound on heat exchange
ΔT_{min}	minimum approach temperature
$\Delta\theta^-, \Delta\theta^+$	scaled deviations from $\boldsymbol{\theta}^0$
Γ	upper bound on the temperature difference

Variables

dth_{ijk}^n	temperature approach for matching (ij) at the hot end of the heat exchanger in stage k at point n
dtc_{ijk}^n	temperature approach for matching (ij) at the cold end of the heat exchanger in stage k at point n
$dtcu_i^n$	temperature approach for matching i and the cold utility at point n
$dthu_j^n$	temperature approach for matching j and the hot utility at point n
F	flexibility index (a scalar)
n_{AS}	number of possible combination of active sets
n_{SN}	number of selected units
n_R	number of rejected (disqualified) networks
q_{ijk}^n	heat exchanged between streams i and j in stage k at point n
qcu_i^n	heat exchanged between stream i and the cold utility at point n
qhu_j^n	heat exchanged between stream i and the hot utility at point n
rrh_{ijk}^n	the hot side heat capacity flow rate used to match z_{ijk} at point n
rh_{ijk}^n	split ratio of hot stream i connected to cold stream j in stage k at point n
rc_{ijk}^n	split ratio of cold stream j connected to hot stream i in stage k at point n
t_{ik}^n	temperature of stream i at the hot end of stage k at point n

t^n_{jk}	temperature of stream j at the hot end of stage k at point n
th^n_{ijk}	temperature for the part of hot i that is connected to cold j in the hot end of an exchanger in stage k at point n
tc^n_{ijk}	temperature for the part of cold j that is connected to hot i in the hot end of an exchanger in stage k at point n
tth^n_{ijk}	temperature for the part of hot i that is connected to cold j in the cold end of an exchanger in stage k at point n
z_{ijk}	binary variable for the existence of a unit for matching stream i and j in stage k
zcu_i	binary variable for the existence of a unit for matching stream i and the cold utility in stage k
zhu_i	binary variable for the existence of a unit for matching stream j and the hot utility in stage k
δ	flexibility (scalar)
Ω	feasible region

Vectors

d	design variables
h	equality constraints
g	inequality constraints
u	control variables
w	state variables
x	variables
z	binary variables
θ	uncertain parameters

REFERENCES

Aaltola, J., "Simultaneous Synthesis of Flexible Heat Exchanger Network," *Appl. Thermal Eng.*, **22**, 907 (2002).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*, Prentice Hall PTR, U.S.A. (1997).

Brooke, A., D. Kendrick., A. Meeraus, R. Raman, and R. E. Rosenthal, *GAMS: A User's Guide*, Scientific Press, Redwood city, U.S.A. (1998).

Chen, J. J. J., "Letter to the Editor: Comments on Improvement on a Replacement for the Logarithmic Mean," *Chem. Eng. Sci.*, **42**, 2488 (1987).

Chen, C. L. and P. S. Hung, "Simultaneous Synthesis of Flexible Heat-Exchange Networks with Uncertain Source-Stream Temperatures and Flow Rates," *I&EC Res.*, **43**, 5916 (2004).

Floudas, C. A., A. R. Ciric, and I. E. Grossmann, "Automatic Synthesis of Optimum Heat Exchanger Network Configurations," *AIChE J.*, **32**, 276 (1986).

Floudas, C. A. and I. E. Grossmann, "Synthesis of Flexible Heat Exchanger Networks with Uncertain Flowrates and Temperatures," *Comput. Chem. Eng.*, **11**, 319 (1987).

Floudas, C. A., *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications*, Oxford Univ. Press: New York, U.S.A. (1995).

Furman, K. C. and N. V. Sahinidis, "A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century," *Ind. Eng. Chem. Res.*, **41**, 2335 (2002).

Grossmann, I. E., K. P. Halemane, and R. E. Swaney, "Optimization Strategies for Flexible Chemical Process," *Comput. Chem. Eng.*, **7**, 439 (1983).

Grossmann, I. E. and C. A. Floudas, "Active Constraint Strategy for Flexibility Analysis in Chemical Processes," *Comput. Chem. Eng.*, **11**, 675 (1987).

Grossmann, I. E., J. A. Caballero, and H. Yeomans, "Mathematical Programming Approaches to the Synthesis of Chemical Process Systems," *Korean J. Chem. Eng.*, **16**, 407 (1999).

Halemane, K. P. and I. E. Grossmann, "Optimal Process Design Under Uncertainty," *AIChE J.*, **29**, 425 (1983).

Konukman, A. E. S., M. C. Camurdan, and U. Akman, "Simultaneous Flexibility Targeting and Synthesis of Minimum-Utility Heat-Exchanger Networks with Superstructure-Based MILP Formulation," *Chem. Eng. Processing*, **41**, 501 (2002).

Linnhoff, B. and E. Hindmarsh, "The Pinch Design Method for Heat Exchanger Networks," *Chem. Eng. Sci.*, **38**, 745 (1983).

Marselle, D. F., M. Morari, and D. F. Rudd, "Design of Resilient Processing Plants–II: Design and Control of Energy Management Systems," *Chem. Eng. Sci.*, **37**, 259 (1982).

Swaney, R. E. and I. E. Grossmann, "An Index for Operational Flexibility in Chemical Process Design. Part I. Formulation and Theory," *AIChE J.*, **31**, 621 (1985).

Yee, T. F., I. E. Grossmann, and Z. Kravanja, "Simultaneous Optimization Models for Heat Integration-I. Area and Energy Targeting and Modeling of Multi-Stream Exchangers," *Comput. Chem. Eng.*, **14**, 1151 (1990).

Yee, T. F. and I. E. Grossmann, "Simultaneous Optimization Models for Heat Integration-II. Heat Exchanger Network Synthesis," *Comput. Chem. Eng.*, **14**, 1165 (1990).

(*Manuscript received Apr. 1, 2005, and accepted Jun. 17, 2005*)

一個考量操作彈性之熱交換器網路合成策略

陳誠亮 郭志豪 洪平松
國立台灣大學化學工程學系

摘 要

本論文提出一個新的熱交換器網路合成策略，所設計的熱交換器網路可以容許程序中各股熱流及冷流的進口溫度及流量在一定範圍之內變動而仍然能維持正常操作。所提出的合成策略可以分成四個步驟進行：

(1) 透過網路超結構，以最小化總年成本為目標，合成一個熱交換器網路；
(2) 暫不考慮各熱交換器之面積限制，針對步驟(1)所得之熱交換器網路做彈性指標分析，測試此結構是否能符合要求的特定操作範圍；
(3) 若(2)分析結果不符合需求，則在限制集合中加入整數切除方程式來限制此結構的使用，並回至步驟(1)，重新進行步驟(1)-(3)直到求得符合要求的熱交換器網路為止，進入步驟(4)；
(4) 考慮熱交換器之面積限制，將步驟(2)所得之熱交換器網路做彈性指標分析，測試此結構是否能符合要求的特定操作範圍，若可則停止，否則需增加熱交換器面積直至符合為止。

在本論文中將透過例子，說明此論文提供之設計策略的效率與可行性。