A SIMULTANEOUS OPTIMIZATION APPROACH FOR SYNTHESIS OF FLEXIBLE HEAT EXCHANGE NETWORKS WITH UNCERTAIN TEMPERATURES AND FLOWRATES

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Abstract

A strategy is proposed for the synthesis of a flexible heat exchange network (HEN) that involves specified uncertainties in the source-stream temperatures and flow rates. The problem is decomposed into three main iterative steps: (1) the simultaneous HEN synthesis to attain a network configuration with a minimum total annual cost (TAC); and (2) the flexibility analysis to test the feasible operation of the network over the full range of uncertain parameters; (3) the exclusion of disqualified networks. For those networks resulting from the synthesis step that are not passing the examination of the flexibility analysis, some integer cuts are appended to forbid reconsidering the disqualified network configurations. A few iterations are required between the synthesis and the flexibility analysis steps. One numerical example is used, demonstrating the efficacy of the proposed flexible HEN synthesis method.

Keywords

Heat exchange network, Synthesis, Flexibility, Superstructure, MINLP

Introduction

The HEN synthesis is by far one of the most developed fields in engineering design. Many techniques including the evolutionary design methods, such as the pinch design method (Linnhoff and Hindmarsh, 1983), and the mathematical programming approaches (Yee and Grossmann, 1990) have been proposed (Grossmann *et. al.*, 1999). A critical review and annotated bibliography for HEN synthesis in the 20th century can be found recently; therein timeline of innovation and major discoveries in HEN synthesis are also addressed by Furman and Sahinidis (2002).

Further to the typical design objective such as the total annual cost, TAC, for the HEN synthesis, the capability of the network for feasible operation under possible variation of input temperatures and flow rates is emphasized in some articles (Floudas and Grossmann, 1987; Aaltola, 2002). Let $P(\delta)$ specify the possible operating range of uncertain parameters, $P(\delta) = \left\{\boldsymbol{\theta} \,\middle|\, \boldsymbol{\theta}^0 - \delta\Delta\boldsymbol{\theta}^- \le \boldsymbol{\theta} \le \boldsymbol{\theta}^0 + \delta\Delta\boldsymbol{\theta}^+\right\}$. $\boldsymbol{\theta}$ is the vector of uncertain parameters (i.e., input temperatures and heat capacity flow rates). $\boldsymbol{\theta}^0$, $\Delta\boldsymbol{\theta}^-$ and $\Delta\boldsymbol{\theta}^+$ are the nominal and the desired negative and positive deviations for these uncertain parameters. The flexible HEN synthesis problem can be defined as synthesizing a network that can be operated for any possible $\boldsymbol{\theta}$ with δ value not less than one. Floudas and Grossmann (1987) propose a novel sequential synthesis method that combines the multi-period mixed-integer linear programming transshipment model for generating the set of stream matches and the nonlinear programming formulation for synthesizing the multi-period networks with the active set strategy of Grossmann and Floudas (1987) for the flexibility analysis. The formulation and synthesis procedure, however, are somewhat tedious for treating the partitioning of temperature intervals under uncertain inlet temperatures. Aaltola (2002) proposes using a multi-period simultaneous MINLP model for minimizing total annual costs and directly generating flexible heat exchange networks. This method seems simple and straightforward since it does not rely on a sequential decomposition. However, the operational feasibility of the resulting network is not guaranteed because only a finite number of operating conditions are considered during design.

In this paper, we are trying to combine the advantages of both approaches by Floudas and Grossmann (1987) and Aaltola (2002) for synthesis of a flexible heat exchange network. An iterative solution strategy, as depicted in Figure 1, is presented for the flexible HEN synthesis problem. The flexible HEN synthesis problem is decomposed into three main iterative steps: the simultaneous HEN synthesis for considering a finite number of operating conditions, the flexibility analysis for testing the feasibility of the network over the full uncertain ranges, and the exclusion of disqualified networks. Further to the finite number of extreme operating conditions to be considered in the synthesis for reducing the searching space,

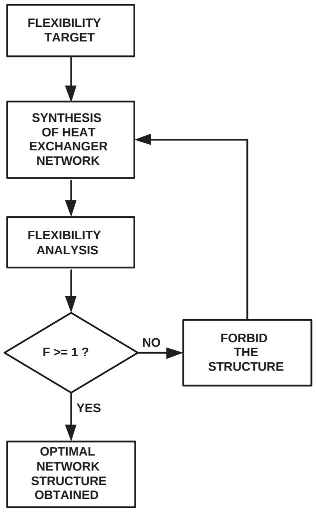

Figure 1: *Proposed strategy for the flexible HEN synthesis*

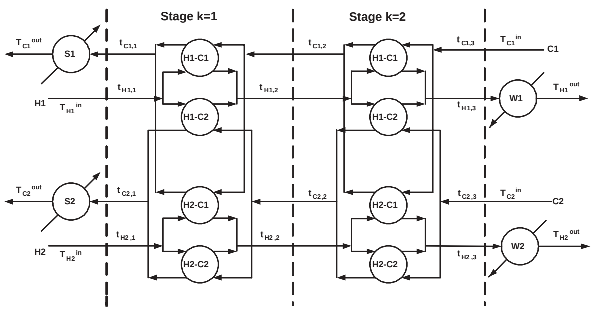

Figure 2: *The two-stage superstructure of Yee and Grossmann*

the desired ranges of operating flexibility, that is, the operable uncertain source-stream temperatures and/or flow rates should be assigned at first. Instead of directly including this flexibility target in the HEN synthesis, the allowable operational range will be evaluated and qualified for a given network structure. The suggested procedure involves the following iterative steps.

Synthesis of Heat Exchange Networks

Consider a HEN synthesis problem with N_H hot streams and N_C cold streams along with hot and cold utilities. The stage-wise superstructure proposed by Yee and Grossmann (1990) is applied for modeling the network structure. The isothermal mixing assumption is also applied to eliminate the need for nonlinear/nonconvex energy balance. Figure 2 illustrates a 2-hot/2-cold/2-stage superstructure for reference. Instead of simultaneously considering the operating flexibility in the synthesis step, a finite number of possible operating vertices are applied to help reducing the searching space. Let $\mathrm{VT} = \{0, 1, \ldots, N_V\}$ denote the index set for multi-periods limiting operating conditions considered for design where index 0 is the nominal one. Suppose the objective function is to minimize the total annual cost, TAC, of the network which includes the average costs of hot and cold utility consumptions over a finite number of operating points and the annualized installation and area costs for the heat exchange units. Then the expanded design variables, $\boldsymbol{x}$, and the reduced feasible searching space, Ω, for the multi-periods formulation of HENS problem can be given as follows (Yee and Grossmann, 1990). Therein LMTD is the log-mean approaching temperature.

$$
\begin{aligned}
&\min_{\boldsymbol{x}\in\Omega} \mathrm{TAC} = \\
&\frac{1}{N_V+1}\left(\sum_{\forall n\in \mathrm{VT}}\sum_{\forall i\in \mathrm{HP}} C_{cu} qcu_i^{(n)} + \sum_{\forall n\in \mathrm{VT}}\sum_{\forall j\in \mathrm{CP}} C_{hu} qhu_j^{(n)}\right) \\
&+ \sum_{\forall i\in \mathrm{HP}}\sum_{\forall j\in \mathrm{CP}}\sum_{\forall k\in \mathrm{ST}} C_{ij}\left[\max_{\forall n\in \mathrm{VT}}\left(\frac{q_{ijk}^{(n)}}{U_{ij}\mathrm{LMTD}_{ijk}^{(n)}}\right)\right] \\
&+ \sum_{\forall j\in \mathrm{CP}} C_{hu,j}\left[\max_{\forall n\in \mathrm{VT}}\left(\frac{qhu_j^{(n)}}{U_{hu,j}\mathrm{LMTD}_{hu,j}^{(n)}}\right)\right] \\
&+ \sum_{\forall i\in \mathrm{HP}} C_{i,cu}\left[\max_{\forall n\in \mathrm{VT}}\left(\frac{qcu_i^{(n)}}{U_{i,cu}\mathrm{LMTD}_{i,cu}^{(n)}}\right)\right]
\end{aligned} \tag{1}
$$

$$
\boldsymbol{x} \equiv \left\{ \begin{array}{r} z_{ijk}, zcu_i, zhu_j; t_{ik}^{(n)}, t_{jk}^{(n)}; \\ dt_{ijk}^{(n)}, dtcu_i^{(n)}, dthu_j^{(n)}; q_{ijk}^{(n)}, qcu_i^{(n)}, qhu_j^{(n)}; \\ \forall\, i\in \mathrm{HP}, j\in \mathrm{CP}, k\in \mathrm{ST}, n\in \mathrm{VT} \end{array} \right\} \tag{2}
$$

$$
\Omega = \left\{ \boldsymbol{x} \;\middle|\; \begin{array}{r}
(T_i^{\mathrm{in}(n)} - T_i^{\mathrm{out}})FCp_i = \sum_{k\in \mathrm{ST}}\sum_{j\in \mathrm{CP}} q_{ijk}^{(n)} \\
+qcu_i^{(n)} \\
(T_j^{\mathrm{out}} - T_j^{\mathrm{in}(n)})FCp_j = \sum_{k\in \mathrm{ST}}\sum_{i\in \mathrm{HP}} q_{ijk}^{(n)} \\
+qhu_j^{(n)} \\
(t_{ik}^{(n)} - t_{i,k+1}^{(n)})FCp_i = \sum_{j\in \mathrm{CP}} q_{ijk}^{(n)} \\
(t_{jk}^{(n)} - t_{j,k+1}^{(n)})FCp_j = \sum_{i\in \mathrm{HP}} q_{ijk}^{(n)} \\
T_i^{\mathrm{in}(n)} = t_{i,1}^{(n)} \\
T_j^{\mathrm{in}(n)} = t_{j,N_T+1}^{(n)} \\
t_{ik}^{(n)} \ge t_{i,k+1}^{(n)},\quad t_{jk}^{(n)} \ge t_{j,k+1}^{(n)} \\
T_i^{\mathrm{out}} \le t_{i,N_T+1}^{(n)},\quad T_j^{\mathrm{out}} \ge t_{j,1}^{(n)} \\
(t_{i,N_T+1}^{(n)} - T_i^{\mathrm{out}})FCp_i = qcu_i^{(n)} \\
(T_j^{\mathrm{out}(n)} - t_{j,1}^{(n)})FCp_j = qhu_j^{(n)} \\
q_{ijk}^{(n)} - \Lambda z_{ijk} \le 0 \\
qcu_i^{(n)} - \Lambda zcu_i \le 0 \\
qhu_j^{(n)} - \Lambda zhu_j \le 0 \\
dt_{ijk}^{(n)} \le t_{ik}^{(n)} - t_{jk}^{(n)} + \Gamma(1 - z_{ijk}) \\
dt_{ij,k+1}^{(n)} \le t_{i,k+1}^{(n)} - t_{j,k+1}^{(n)} + \Gamma(1 - z_{ijk}) \\
dtcu_i^{(n)} \le t_{i,N_T+1}^{(n)} - T_{\mathrm{CU}}^{\mathrm{out}} + \Gamma(1 - zcu_i) \\
dthu_j^{(n)} \le T_{\mathrm{HU}}^{\mathrm{out}} - t_{j,1}^{(n)} + \Gamma(1 - zhu_j) \\
dt_{ijk}^{(0)}, dtcu_i^{(0)}, dthu_j^{(0)} \ge \Delta T_{min} \\
z_{ijk}, zcu_i, zhu_j \;\in\; \{0,1\} \\
t_{ik}^{(n)}, t_{jk}^{(n)}, q_{ijk}^{(n)}, qcu_i^{(n)}, qhu_j^{(n)} \;\ge\; 0 \\
dt_{ijk}^{(n)}, dtcu_i^{(n)}, dthu_j^{(n)} \;\ge\; 0 \\
i\in \mathrm{HP}, j\in \mathrm{CP}, k\in \mathrm{ST}, n\in \mathrm{VT}
\end{array} \right\} \tag{3}
$$

Flexibility Analysis

Solution of Eq.(1) results in a heat exchange network of minimal TAC with specific configuration that satisfies multiple extreme operating conditions. The resilience of the resulting network to full range of uncertainties in the source-stream temperatures and flow rates can be measured by the flexibility index proposed by Swaney and Grossmann (1985). The physical performance of a chemical process can be described by the following set of constraints

$$\begin{aligned} \boldsymbol{h}(\boldsymbol{d},\boldsymbol{u},\boldsymbol{w},\boldsymbol{\theta}) &= 0 \\ \boldsymbol{g}(\boldsymbol{d},\boldsymbol{u},\boldsymbol{w},\boldsymbol{\theta}) &\leq 0 \end{aligned} \tag{4}$$

where $\boldsymbol{h}$ is the vector of equation which hold for steady-state operation of the process, and $\boldsymbol{g}$ is the vector of inequalities which must be satisfied if operation is to be feasible. The variables are classified into four categories in these equations. Therein $\boldsymbol{\theta}$ is the vector of uncertain parameters (*i.e.* temperatures and flow rates). The design variables $\boldsymbol{d}$, obtained from the synthesis step, define the network structure and the sizes of the heat exchange units. The control variables $\boldsymbol{u}$ stands for the degrees of freedom during the operation of the network. $\boldsymbol{w}$ is the state variables, which can be expressed as implicit functions of control variables $\boldsymbol{u}$ and uncertain parameters $\boldsymbol{\theta}$ by solving the equality constraints.

$$\boldsymbol{h}(\boldsymbol{d},\boldsymbol{u},\boldsymbol{w},\boldsymbol{\theta}) = 0 \Rightarrow \boldsymbol{w} = \boldsymbol{w}(\boldsymbol{d},\boldsymbol{u},\boldsymbol{\theta}) \tag{5}$$

Thus the inequalities of the network can be represented by the following forms where $\boldsymbol{M}$ is the index set of reduced independent inequalities.

$$g_m\left[\boldsymbol{d},\boldsymbol{u},\boldsymbol{w}(\boldsymbol{d},\boldsymbol{u},\boldsymbol{\theta}),\boldsymbol{\theta}\right] = f_m(\boldsymbol{d},\boldsymbol{u},\boldsymbol{\theta}) \leq 0 \qquad \forall m \in \boldsymbol{M} \tag{6}$$

Then the flexibility index problem of a network can be formulated as the following mixed-integer nonlinear programming problem by Grossmann and Floudas (1987) to account for the possibility of non-extreme critical points. The mathematical details can be found elsewhere.

$$\begin{aligned} \mathcal{F} = & \min_{\boldsymbol{\theta},\boldsymbol{u},s_m,\lambda_m,y_m,\delta} \delta \\ \text{s.t.} \quad & s_m + f_m(\boldsymbol{d},\boldsymbol{u},\boldsymbol{\theta}) = 0 \\ & \left.\begin{aligned} \sum_{\forall m\in \boldsymbol{M}} \lambda_m \frac{\partial f_m}{\partial \boldsymbol{u}} &= 0 \\ \sum_{\forall m\in \boldsymbol{M}} \lambda_m &= 1 \\ \lambda_m - y_m &\leq 0 \end{aligned}\right\}\star \\ & s_m - V(1-y_m) \leq 0 \\ & \sum_{m\in \boldsymbol{M}} y_m = n_u + 1 \\ & \boldsymbol{\theta}^{(0)} - \delta\Delta\boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^{(0)} + \delta\Delta\boldsymbol{\theta}^+ \\ & y_m \in \{0,1\} \\ & \delta, \lambda_m, s_m \geq 0, \ \forall m \in \boldsymbol{M} \end{aligned} \tag{7}$$

In these equations, $\mathcal{F}$ represents quality of flexibility level where an $\mathcal{F}$ value not less than one means the network is 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 large enough real number; n_u is the number of control variables $\boldsymbol{u}$. Details of the above MINLP formulation can be found in the literatures (Grossmann and Floudas, 1987).

For the solution of the mixed-integer optimization problem, Eq.(7), the Active Set Strategy consists of three basic steps (Floudas and Grossmann, 1987). At first, the candidate active sets should be identified. Let $\mathrm{N_{AS}} = \{1, \cdots, n_{\mathrm{AS}}\}$ denote the index set of all possible combinations for the active constraints, and $\mathrm{AS}(k)$ represent the k^{th} index set of active constraints. Then a value of δ^k for the k^{th} candidate active set can be obtained by solving the following nonlinear programming NLP problem (Floudas and Grossmann, 1987):

$$\begin{aligned} \delta^k &= \min_{\boldsymbol{\theta},\boldsymbol{u},\delta} \delta \\ \text{s.t.} \quad f_m(\boldsymbol{d},\boldsymbol{u},\boldsymbol{\theta}) &= 0 \\ \boldsymbol{\theta}^{(0)} - \delta\Delta\boldsymbol{\theta}^- \leq \ \boldsymbol{\theta} & \leq \boldsymbol{\theta}^{(0)} + \delta\Delta\boldsymbol{\theta}^+ \\ \delta &\geq 0 \\ \forall m &\in \mathrm{AS}(k) \subseteq \boldsymbol{M} \end{aligned} \tag{8}$$

The solution of the Flexibility Index problem is given by:

$$\mathcal{F} = \min_{\forall k \in \mathrm{N_{AS}}} \delta^k \tag{9}$$

Notice that for those problems where there is no control variable (*i.e.,* $n_u = 0$), the flexibility analysis problems would become much simpler (Grossmann and Floudas, 1987). In such a case the stationary conditions in Eq.(7), that is, the three relations marked with $\star$ and the associated Kuhn-Tucker multipliers $\lambda_m' s$, can be eliminated. In this reduced formulation only one constraint is allowed to be active for each active set. Eq.(7) can thus be decomposed in terms of each individual constraint, that is, $\mathrm{AS}(k) = \{k\}, \forall k \in \mathrm{N_{AS}}$. The flexibility index problem can thus be simplified significantly.

Integer Cuts to Exclude Disqualified Networks

The flexibility index of the network resulting from the synthesis step is evaluated to check if the current network satisfies the previously assigned flexibility target, that is, whether the network can be operated over the full range of possible input stream temperatures and flow rates. All of the disqualified networks will be excluded in the updated synthesis work. There are two cases to guarantee possession of a new network structure: (1) At least one currently rejected unit in a disqualified network is selected; or (2) Current selections of a disqualified network are not all chosen again. Case 1 gives a new HEN since it includes at least one new unit compared with the forbidden one, no matter if those currently selected units are all chosen again or not. Whereas case 2 also gives a new HEN since some units in charge currently are excluded, no matter the currently declined units are picked up or not. Suppose there are total N_{A} abandoned networks and let SN^{ℓ} and RN^{ℓ} denote index sets of selected units and rejected units of the ℓ^{th} abandoned HEN, respectively, and N_{SN}^{ℓ} denote the total number of selected units of the ℓ^{th} abandoned HEN. Then the

the operating cost (OC), the total annual cost (TAC), and the flexibility of resulting networks for example 1

	ACC	OC	TAC	$\mathcal{F}$
Simultaneous	$30,104$	$11,772$	$41,876$	1.7134
Sequential	$39,380$	$10,499$	$49,879$	1.0

above two cases can be respectively expressed by the following logic constraints:

$$\begin{aligned} &\text{Case 1:} \quad \sum_{\forall z \in \text{RN}^\ell} z \geq 1 \quad \text{and} \quad \sum_{\forall z \in \text{SN}^\ell} z \leq N_{\text{SN}}^\ell \\ &\text{Case 2:} \quad \sum_{\forall z \in \text{RN}^\ell} z \geq 0 \quad \text{and} \quad \sum_{\forall z \in \text{SN}^\ell} z < N_{\text{SN}}^\ell \\ &\qquad\qquad\qquad\qquad\qquad\qquad \ell = 1, \cdots, N_{\text{A}} \end{aligned} \tag{10}$$

Define new binary variable z_d^ℓ to denote these two acceptable conditions, *i.e.*, $z_d^\ell = 1$ for case 1 and 0 for case 2. Then the above two logic constraints can be expressed as follows,

$$\begin{aligned} \sum_{\forall z \in \text{RN}^\ell} z &\geq z_d^\ell \\ \sum_{\forall z \in \text{SN}^\ell} z &\leq N_{\text{SN}}^\ell - 1 + z_d^\ell \\ z_d^\ell &\in \{0, 1\}, \quad \ell = 1, \cdots, N_{\text{A}} \end{aligned} \tag{11}$$

There two expressions can be further combined into the following integer cut.

$$\sum_{\forall z \in \text{SN}^\ell} z - \sum_{\forall z \in \text{RN}^\ell} z \leq N_{\text{SN}}^\ell - 1, \;\; \ell = 1, \cdots, N_{\text{A}} \tag{12}$$

With these integer cuts appended into the constraints in the synthesis step, one can obtain a new candidate network with a configuration different to all previously abandoned networks. Several iterations may sometimes be required between the network synthesis and the flexibility analysis steps for reaching the qualified configuration. One numerical example modified from Floudas and Grossmann (1987) will be used to demonstrate the efficiency of proposed flexible HEN synthesis method.

Numerical Example

The example involves two hot and two cold streams ($N_H = 2$, $N_C = 2$) along with steam and cooling water as heating and cooling utilities. The problem data is presented in Floudas and Grossmann (1987). The minimum number of superstructure stages, N_T, is selected as two corresponding to $\max\{N_H, N_C\} = 2$, and suppose capital annualization factor is 0.2. The HEN synthesis results are shown in Table 1 and Figure 3.

Conclusion

In this paper, a new strategy has been proposed to synthesize a flexible heat exchange network that involves uncertain source-stream temperatures and flow rates. Several iterations may be required to determine the qualified network. One numerical example is supplied, demonstrating that the proposed strategy can provide a network flexible for operation within assigned variations in input temperatures and/or flow rates.

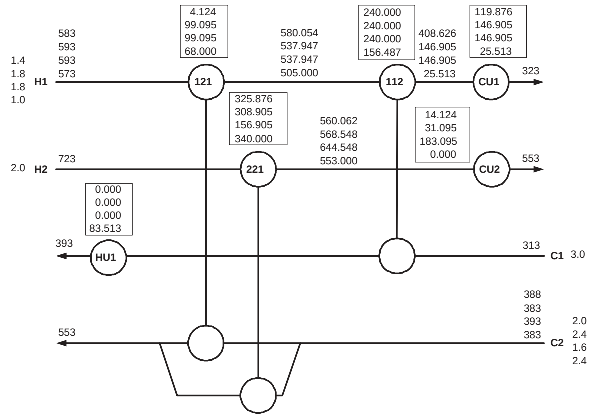

Figure 3: *HEN structures for example* 1 *when considering nominal with periods* $1 \sim 3$ *for synthesis*

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