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## Article

# Heat exchanger network synthesis integrated with flexibility and controllability<sup>☆</sup>

Siwen Gu, Linlin Liu, Lei Zhang, Yiyuan Bai, Shaojing Wang, Jian Du<sup>\*</sup>

Institute of Chemical Process Systems Engineering, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, China

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## ABSTRACT

Over the last three decades, flexibility and controllability considerations for heat exchanger networks (HENs) have received great attention, respectively. However, they should be simultaneously incorporated in HEN synthesis to allow the economic performance to be achievable in a practical operating environment. This paper proposes a method for simultaneous synthesis of flexible and controllable HEN by considering their coupling. The key idea is to add the bypasses with optimized initial fractions and positions to explore such coupling, and consequently enabling HENs to be operated successfully over a range of disturbance variations. These are implemented by identifying and quantifying disturbance propagations, and then examining the sensitivity of bypasses to the entire HEN. In this way, the superstructure-based mixed integer non-linear programming (MINLP) with objective function of minimizing the total annual cost is formulated. A case study is used to demonstrate the application of the proposed method. Quantitative measures and dynamic simulation show the ability to provide the satisfactory flexibility and controllability of the obtained HEN.

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## 1. Introduction

The synthesis of heat exchanger networks (HENs) plays a crucial role in the overall chemical process. The main aim of the synthesis is to find a HEN with minimum total annual cost. Several synthesis methods with different features have been proposed in the literatures, such as: 1) applied to large-scale HENs: Chen *et al.* [1] and 2) focusing on continuous processes with batch streams: Wang *et al.* [2]. These synthesis methods are performed under the assumption of fixed operating parameters at nominal conditions. However, the environment may introduce significant changes in the operating conditions. To ensure feasibility and optimality of operation, therefore, flexibility and controllability should be simultaneously considered in HEN synthesis.

As a fundamental requirement of HENs for maintaining feasibility, flexibility problems have been researched extensively in the literatures. For flexibility analysis, Swaney and Grossmann [3] proposed a flexibility index, which defined the maximum parameter range achievable for a feasible operation. Subsequently, based on such flexibility analysis, the flexible HEN synthesis aims to

enable it to have the capability of withstanding the expected disturbances. Numerous works have appeared in the literatures throughout the past years. Based on a multiperiod superstructure representation, Papalexandri and Pistikopoulos [4] proposed a HEN retrofit strategy for improving the flexibility. Li *et al.* [5] proposed a method for synthesizing flexible HENs, which was sequentially implemented by two main steps: structure synthesis and area optimization. To improve the dynamic flexibility of batch processes, Zhou *et al.* [6] proposed a method based on optimizing the initial operating condition. However, it was the assumed that all degree of freedom was able to be adjusted during the whole period of operation. Also, the manipulated variables (MVs) were assumed to take complete control of the controlled variables (CVs). This may lead to difficulties for achieving the optimal operation in the presence of disturbances.

Moreover, strong interaction exists in the streams due to the combinatorial nature of HENs. This also will significantly increase the difficulties of achieving the optimal operation under disturbances. To address these problems, review papers that summarize the different ways and the development in the area of integrated design and control are available [7–9]. However, it is still essential to reduce the potential difficulties in control designs, as discussed in controllability problems. That is, in this work the term controllability means how easy the HEN is to control [10,11]. And controllability is strongly dependent on both the control structure and the

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<sup>\*</sup> Corresponding author.

E-mail address: [dujian@dlut.edu.cn](mailto:dujian@dlut.edu.cn) (J. Du).

HEN configuration [10]. Firstly, as for a given HEN, each CV is paired with one MV and each pairing defines a control loop, and then the control structure is formed by the whole set of control loops. For this purpose, the control structure design has received considerable attentions. Several methods based on the relative order have been proposed in the literatures, in which is a structure measure of how direct an effect a MV has on a CV [12]. For simplicity Lersbamrungsuk *et al.* [12] assumed relative order as a number of heat exchangers between CV and MV, and then proposed the control structure design method. Kang *et al.* [13] extended their works to propose a control structure design method in a graph theoretic setting. Recent reviews in this area can be found in Kookos and Perkins [14] and Braccia *et al.* [15].

Another important issue particularly relevant to controllability problems is the synthesis of controllable HEN, which is a prerequisite for designing control structures. As far back as in 1992, Huang and Fan [16] devoted an entire paper to incorporate controllability analysis in the HEN synthesis, by the means of identifying and quantifying disturbance propagations in the HEN. However, as the disturbances were classified into three degrees of intensity and then the quantification of disturbance propagation was based on approximate reasoning, the method might introduce noticeable errors for some cases, and the solutions might not be preferable when more precise process evaluation is needed [17]. Most recent works have developed the process synthesis method based on their work, such as, 1) giving four heuristic rules: Shoaib [18] and 2) for shortest disturbance propagation path: Hafizan *et al.* [19]. On the other hand, the optimization for the position of the MVs by the sensitivity analysis is also employed for considering the controllability in the HEN synthesis. In the work of Papadopoulos *et al.* [20], the sensitivity-based investigation provided useful insights into the integration of solvent and process design with controllability consideration.

According to the above analyses, the control structure design, the disturbance propagation identification and quantification are introduced to reduce the potential difficulties of control designs. Besides, this goal can also be achieved by ensuring sufficient controlled operation space for HENs, which can be provided through the optimization of the initial bypass fractions [21]. The need to consider bypass fractions in control designs has been widely accepted. Uztürk and Akman [22] suggested that the upper and lower bounds of bypass fractions should be investigated for considering the realizability of the HEN control. As for the control design of a given HEN, Giovanini and Marchetti [23] suggested that a bypass whose initial fraction was equal to zero was activated only if the auxiliary variable was included. However, the HEN synthesis considering initial bypass fractions is particularly desirable in keeping the optimal energy integration in a practical operating environment. Luo *et al.* [21] presented a margin optimization design method for HENs with bypasses and the desired fractions were obtained on the basis of satisfying process conditions. The bypass fractions were obtained by offline calculation and did not consider disturbances.

In summary, the flexibility and controllability are strongly affected by the HEN synthesis. It is crucial to have in mind that a HEN must not only keep the economically optimal energy integration, but also exhibit flexibility and controllability that will allow this economic performance to be achievable in a practical operating environment. Escobar *et al.* [10] proposed a framework for implementing the synthesis of flexible and controllable HENs. A multiperiod synthesis of HENs was employed to improve the HEN flexibility, and then a control structure was designed with the objective of minimizing the control loop interaction and the disturbance sensitivity. However, the internal trade-offs, *i.e.* the coupling between flexibility and controllability, were not adequately processed. This imposes restrictions on optimization abil-

ity, and consequently often leads to suboptimal solutions under global objective.

This paper investigates the incorporation of flexibility and controllability in the HEN synthesis. Considering their coupling, a method is presented to synthesize HENs while achieving flexibility and controllability simultaneously. The key idea is to add the bypasses with optimized initial fractions and positions to explore the coupling, and consequently maintaining feasibility and optimality of operation in the presence of the disturbances. This work begins with the identification and quantification of disturbance propagations, which are employed to optimize the initial fractions of all the potential bypasses. Then, the sensitivity factors are defined to examine their sensitivity to the entire HEN in order to optimize bypass positions. A superstructure-based mixed integer non-linear programming (MINLP) model with objective function of minimizing the total annual cost is formulated. With the proposed method, a HEN not only is economically optimal, but also exhibits the satisfactory flexibility and controllability.

## 2. Problem Statement

The aim of this paper is to synthesize a HEN with minimum total annual cost that is able to operate feasibly under disturbances. The problem to be addressed can be stated as follows. Given are: (1) the stream data, (2) a specified range for the expected disturbances, *i.e.* inlet stream temperatures and heat capacity flowrates, and (3) a minimum temperature approach ( $\Delta T_{\min}$ ). The following general assumptions are related to this work: (1) pressure drop and further fluid dynamics considerations are neglected; (2) bypass fractions are regarded as MVs; (3) utility duties may be employed for control purposes (potential MVs); and (4) the stream output temperatures are regarded as the CVs.

## 3. Mathematical Formulation

### 3.1. Method for simultaneous synthesis of flexible and controllable HENs

In the previous methods, flexibility and controllability considerations in the HEN synthesis were isolated to some extent, so that the internal trade-offs were not adequately processed. Such stepwise nature imposes restrictions on optimization ability, and consequently often leads to suboptimal solutions under global objective. In contrast, this paper is devoted to simultaneously synthesize flexible and controllable HEN by considering the coupling between the flexibility and controllability.

To improve HEN flexibility, the increases in the heat exchanger areas, the numbers of new units and bypasses can be found in the previous works, such as Papalexandri and Pistikopoulos [4] and Li *et al.* [5]. Once the HEN is flexible, in order to operate this HEN, the controllability must be ensured. As bypasses can be regarded as sinks for disturbances, we can also improve the controllability with respect to disturbance rejection by adding bypasses. Hence, it is crucial to optimize the positions of bypasses in HEN synthesis for both improving flexibility and controllability. On the other hand, depending on the directions of the expected disturbances, some disturbances may be rejected only by decreasing bypass fractions, and if some or all initial bypass fractions are zero, the HEN may not have the controlled operation space and the capability of accommodating the disturbances as much as desired. Hence, the optimization of initial bypass fractions in HEN synthesis can be employed to explore how direct an effect a disturbance has on a HEN, and subsequently, achieving the trade-off among the total expenditure, the controlled operation space and the capability of accommodating disturbances of the HEN. Moreover, the bypass

fraction and position are two key elements that facilitate the HEN synthesis considering bypasses through the use of the optimization method. In this way, the coupling between flexibility and controllability can be reflected by adding the bypasses with optimized initial fractions and positions, and consequently their simultaneous consideration in HEN synthesis can be implemented.

The proposed method can be seen as an extension of the work of Shoaib [18], in which controllability is explicitly considered in HEN synthesis by identifying and quantifying disturbance propagations. However, the connotation of each step is different, as well as the method. Firstly, these are both employed to implement the optimization of the initial fractions of all the possible bypasses so as to explore how direct an effect a disturbance has on a HEN. Secondly, for ensuring both the controlled operation space and the capability of accommodating disturbances, the disturbance propagations from the disturbance sources to the sinks are identified by the proposed heuristic rules. Another major difference is we propose a disturbance index to quantify the disturbance propagation, which is regarded as the number of the heat exchangers in an identified disturbance propagation. It is a structure measure of how direct an effect a disturbance source has on a disturbance sink. Furthermore, the optimization in the positions of bypasses with optimized initial fractions is implemented by examining their sensitivity to the entire HEN so as to improve flexibility and controllability with respect to disturbance rejection.

The flowchart of the proposed method is denoted in Fig. 1. The procedure starts with the given stream data. Based on the identifi-

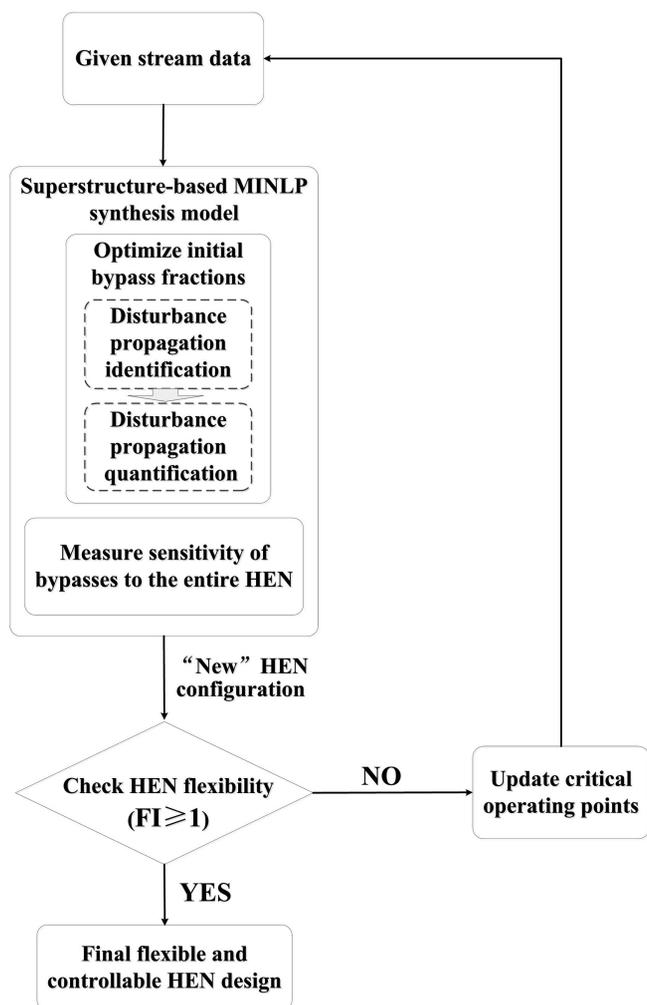


Fig. 1. Flowchart of the proposed method.

cation of disturbance propagations, the quantification is involved for optimizing the initial fractions of all the potential bypasses. And then their sensitivity to the entire HEN is analyzed for optimizing the bypass positions. The constraint related to the number of bypasses is also observed. In this way, a superstructure-based MINLP with objective function of minimizing the total annual cost is formulated, so that a HEN is obtained while determining the bypasses with optimized initial fractions and positions. The superstructure is similar to the one proposed by Yee *et al.* [24], which includes all the possible bypasses, as illustrated in Fig. 2. Subsequently, HEN flexibility is examined by the flexibility index and its calculation method is referred to Li *et al.* [25]. If there does not exist much flexibility, *i.e.* the flexibility index is smaller than 1, the critical operating points will be found by the flexibility analysis which is referred to Li *et al.* [5,25]. They will be added to the nominal conditions and the synthesis problem will be solved again.

### 3.2. Initial bypass fractions

The disturbances and control requirements are inseparable from the HEN synthesis, thereby rendering the desired capability of accommodating disturbances and the reduced difficulties in control designs essentially impossible. As discussed in the work of Huang and Fan [16], the HEN experienced different disturbance intensity and required different control actions given by bypasses. However, the information on these is imprecise, incomplete and uncertain, especially for the difference originating various disturbances. As these disturbances propagate through the HEN and may result in offsets in stream output temperatures, downstream-path is employed to give insight into the identification for disturbance propagations [16]. This paper proposes three heuristic rules to identify disturbance propagations. And then the quantification is implemented by the numbers of heat exchangers in the identified disturbance propagations. Such disturbance intensity is defined as a disturbance index. Subsequently, the optimization of initial bypass fraction is associated with the following logical statement: wide controlled operation space is assigned to the bypass with large disturbance intensity.

#### 3.2.1. Disturbance propagation identification

The disturbances originating from the sources propagate essentially through their downstream-paths [16]. Such downstream-path involves the specific heat exchangers and then the variations in these heat exchangers (*e.g.* the variations of output temperatures of the heat exchangers) reflect the effects of disturbances on the HEN. Therefore, the disturbance propagation is strongly dependent on the HEN configuration. Two possible disturbance propagations from an inlet stream temperature to a stream output temperature are established to express the connection between the disturbance propagation and the HEN configuration. As shown in Fig. 3, there is only heat exchanger HE2 in DP 2 propagating from the inlet temperature of stream H1 to the output temperature of stream C1. So the disturbances in DP 2 will not directly propagate to other streams and the disturbance intensity is also not influenced by other heat exchangers/streams. Whereas that of the output temperature of stream H2 may be varied by the heat exchangers in DP 1. This is due to the fact that they are associated with other streams. In summary, as a heat exchanger may correspond to different disturbance propagations, the more heat exchangers in the disturbance propagations there are, the larger effects of disturbances on the stream output temperatures there exist, the broader controlled operation space with respect to bypass adjustments needed is.

As discussed above, each bypass adjustment for control purposes is mainly associated with the disturbance propagations. Therefore, the disturbance propagation has to be developed for

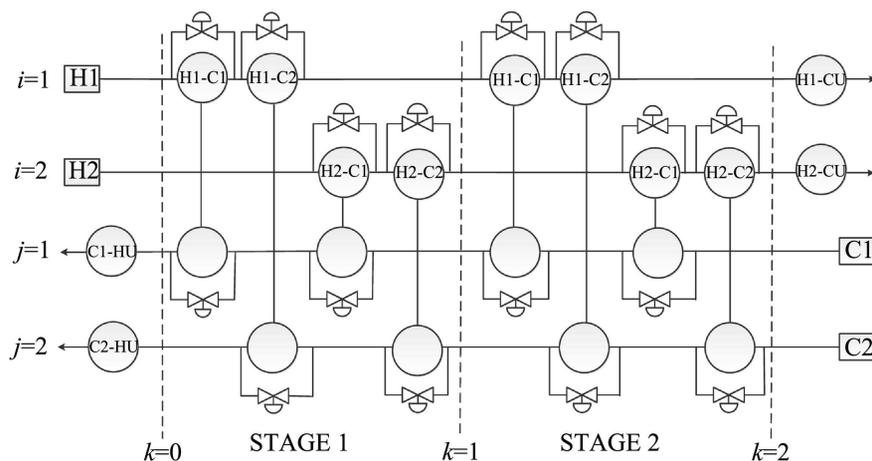


Fig. 2. Non-split two-stage superstructure of heat exchanger networks involving all the possible bypasses.

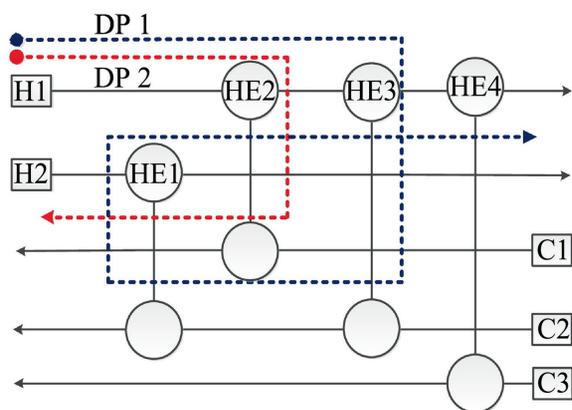


Fig. 3. Two possible disturbance propagations.

each bypass which is regarded as a disturbance sink. And all the possible disturbances are assigned to each heat exchanger, so that a heat exchanger is regarded as a disturbance source. The disturbance loops are defined to describe the disturbance propagation from the heat exchangers to the bypasses. Moreover, the identification of the disturbance propagations is required to implement in the superstructure to take into account all the possibilities. According to the above analyses, the heuristic rules for the disturbance propagation identification are listed below:

- (1) The disturbance propagation along the heat exchangers in the same stream is not considered.
- (2) The disturbance propagation from one stream side of a heat exchanger to a bypass placed in the other side of this heat exchanger is not involved.
- (3) When there exist the same numbers of heat exchangers in different disturbance loops, the one including the heat exchangers in the upstream of the relevant bypasses is considered as a priority.

When the disturbances propagate in a stream, the relevant disturbance intensity will feature more stable than other possible disturbance propagations. Hence, it is assumed that the disturbance propagation in a stream can be ignored, as discussed in Rule 1.

### 3.2.2. Disturbance propagation quantification

The effect of any of the disturbances on the HEN depends on the distances of the disturbance sources from the disturbance sinks.

Lersbamrungsuk *et al.* [12] discussed the number of the heat exchangers placed between a MV and a CV, giving an idea of the disturbance propagation quantification. In this paper, the key to such quantification is the number of the heat exchangers within an identified disturbance loop. For disturbance loop  $s$ , the disturbance intensity in bypass  $l$  is described below:

$$N_{l,s} = z_{ijk,s}^f \cdot z_{ijk,s}^c \cdot z_{ijk,s}^{la} \left( n_{ijk,s}^{f,side} \cdot z_{ijk,s}^f + n_{ijk,s}^{c,side} \cdot z_{ijk,s}^c + n_{ijk,s}^{m,side} \cdot z_{ijk,s}^m + n_{ijk,s}^{la,side} \cdot z_{ijk,s}^{la} \right) \quad (1)$$

where  $N_{l,s}$  is defined as the disturbance index of bypass  $l$ . This index only corresponds to the disturbance intensity propagated from the heat exchangers in disturbance loop  $s$ . Therefore, considering all the disturbance loops, the disturbance intensity in bypass  $l$  is the summation of the disturbance indexes with  $\sum_s N_{l,s}$ ,  $L = \{1, 2, \dots, l\}$  is

the set of the bypasses.  $HL = \{1, 2, \dots, hl\}$  and  $CL = \{1, 2, \dots, cl\}$  are subsets of  $L$ , denoting the bypasses in hot and cold sides of the heat exchangers, respectively. These correspond to the set of the heat exchangers with  $F = \{111, 121, \dots, ijk\}$  obtained by the above superstructure. Where the subscripts  $i, j$  and  $k$  denote hot, cold streams and the stages, respectively. The heat exchanger with  $ijk$  indicates the stream match between hot stream  $i$  and cold stream  $j$  in stage  $k$ . Besides, first, last and crucial heat exchangers are defined to denote the existence of the disturbance loop  $s$ , which are expressed by superscripts  $f, la$  and  $c$ , respectively. And a middle heat exchanger is proposed to introduce disturbances on this disturbance loop but little effect on its existence, which is denoted by superscript  $m$ . Binary variables  $z_{ijk,s}^f, z_{ijk,s}^c, z_{ijk,s}^m$  and  $z_{ijk,s}^{la}$  denote the existence of the four heat exchangers, respectively. Taking  $z_{ijk,s}^f$  as an example:

$$z_{ijk,s}^f = \begin{cases} 1, & \text{if first heat exchanger exists} \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

Besides, in Eq. (1),  $n_{ijk,s}^{f,side}, n_{ijk,s}^{c,side}, n_{ijk,s}^{m,side}$  and  $n_{ijk,s}^{la,side}$  refer to the affected stream sides of the heat exchangers in disturbance loop  $s$  caused by disturbance propagations.

### 3.2.3. Optimization for initial bypass fractions

If the disturbance propagation is severe, the HEN may not be operable regardless of the advance of control techniques. To prevent this occurrence, the HEN should be able to reject severe disturbance propagation. That is, its controlled operation space should be broadened. For this purpose, this desired controlled operation space is realized through optimizing the initial fractions of all the potential bypasses.

According to the above sections, the greater disturbance indexes are assigned to the bypasses experiencing more severe disturbance propagations. This implies that the wider controlled operation space has to be considered by optimizing the initial fractions of these bypasses. For this purpose, the middle value of the bypass fraction is involved, which is associated with the following logical statement: great disturbance intensity in a bypass implies small difference between this bypass fraction and its middle value. Furthermore, all the disturbance propagations will impose large effects on the heat exchangers located at the end of the streams, thereby the bypasses placed in these heat exchangers should have the wider controlled operation space. These are employed to determine the initial fractions of all the potential bypasses, which are enforced by the following constraints:

$$f^{H,\text{end}}(N, K^H, K^{H,\text{md}}) - f_o^H(N, K^H, K^{H,\text{md}}) \geq 0 \quad (3)$$

$$f^{C,\text{end}}(N, K^C, K^{C,\text{md}}) - f_o^C(N, K^C, K^{C,\text{md}}) \geq 0 \quad (4)$$

where  $f$  denotes the product of the disturbance intensity in a bypass and the difference with the middle value of this bypass fraction.  $f^{H,\text{end}}$  and  $f^{C,\text{end}}$  are the products corresponding to the bypasses in the heat exchangers that are closest to the end of the streams. Accordingly,  $f_o^H$  and  $f_o^C$  are the products corresponding to the bypasses in other heat exchangers in this stream.  $o$  is the set of these heat exchangers in this stream with  $O = \{1, 2, 3\}$ . Taking the heat exchangers in stream  $i$  as an example, when the heat exchanger with  $ijk$  is closest to the end of stream, the relationship between the bypass  $hl$  in the hot side of this heat exchanger and the bypass  $hl - 1$  in the hot side of the possible adjacent heat exchanger is given by:

$$\sum_s N_{hl,s} \cdot |K_{ijk}^H - K_{ijk}^{H,\text{md}}| - \sum_s N_{(hl-1),s} \cdot |K_{i(j-1)k}^H - K_{i(j-1)k}^{H,\text{md}}| \geq 0 \quad (5)$$

where  $K_{ijk}^H$  is the bypass fraction and  $K_{i(j-1)k}^H$  is that of the possible adjacent heat exchanger.  $K_{ijk}^{H,\text{md}}$  and  $K_{i(j-1)k}^{H,\text{md}}$  are the middle values of the corresponding bypass fractions.

### 3.3. Sensitivity measure for bypasses

As discussed in the previous sections, it is crucial to optimize the positions of the bypasses with optimized initial fractions in HEN synthesis for both improving flexibility and controllability. In terms of both the disturbance rejection and the capability of accommodating disturbances, the bypasses that are expected to take complete control of the corresponding stream output temperatures can introduce the positive effect on the flexibility and controllability of this HEN. Hence, a bypass that is more sensitive to all the stream output temperatures is added in the HEN, and consequently the possibility of achieving the satisfactory flexibility and controllability will be increased. In this way, the sensitivity factor is proposed to describe the sensitivity of a bypass to all the stream output temperatures, as well as the entire HEN.

Due to the combinatorial nature of HENs, the sensitivity factor can be introduced by the heat balances of the streams and the heat exchangers. In this way, the situation in which the heat duty of a stream is the summation of that of the heat exchangers in this stream is employed to establish the relationship of a bypass with all the streams. Taking the heat balance of hot stream  $i$  as an example:

$$Qh_i = \sum_j \sum_k Q_{ijk}^{\text{HE}} \quad (6)$$

where  $Qh_i$  is the heat duty of hot stream  $i$ .  $Q_{ijk}^{\text{HE}}$  is the heat duty of a heat exchanger, which is expressed with:  $Q_{ijk}^{\text{HE}} = 0.5(Qh_{ijk}^{\text{HE}} + Qc_{ijk}^{\text{HE}})$ . Where  $Qh_{ijk}^{\text{HE}}$  and  $Qc_{ijk}^{\text{HE}}$  are the heat duties of stream sides of heat

exchangers. It is noted that the aforementioned descriptions are employed to make the bypasses more closely linked with all the heat exchangers and stream output temperatures. Therefore, the heat balances are extended to describe the sensitivity factors of the bypasses:

$$\frac{\partial Th_i^{\text{OUT}}}{\partial K_{ijk}^H} = \frac{\partial Qh_i}{\partial K_{ijk}^H} \left( \frac{\partial Qh_i}{\partial Th_i^{\text{OUT}}} \right)^{-1}, \quad \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{ijk}^H} = \frac{\partial Qc_j}{\partial K_{ijk}^H} \left( \frac{\partial Qc_j}{\partial Tc_j^{\text{OUT}}} \right)^{-1} \quad (7)$$

$$\frac{\partial Th_i^{\text{OUT}}}{\partial K_{ijk}^C} = \frac{\partial Qh_i}{\partial K_{ijk}^C} \left( \frac{\partial Qh_i}{\partial Th_i^{\text{OUT}}} \right)^{-1}, \quad \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{ijk}^C} = \frac{\partial Qc_j}{\partial K_{ijk}^C} \left( \frac{\partial Qc_j}{\partial Tc_j^{\text{OUT}}} \right)^{-1} \quad (8)$$

where the sensitivity factors are defined with  $\omega_{hl}^H = \{\partial Th_i^{\text{OUT}}/\partial K_{ijk}^H, \partial Tc_j^{\text{OUT}}/\partial K_{ijk}^H\}$  and  $\omega_{cl}^C = \{\partial Th_i^{\text{OUT}}/\partial K_{ijk}^C, \partial Tc_j^{\text{OUT}}/\partial K_{ijk}^C\}$ .  $\omega_{hl}^H$  and  $\omega_{cl}^C$  denote the sensitivity factors of bypasses to all the stream output temperatures.  $Th_i^{\text{OUT}}$  and  $Tc_j^{\text{OUT}}$  are the output temperatures of hot stream  $i$  and cold stream  $j$ , respectively. A bypass has  $i + j$  sensitivity factors, resulting in a sensitivity factor matrix. The sensitivity factor matrices regarding the bypasses in the hot and cold sides of the heat exchangers are described as follows:

$$[\omega_1^H \ \dots \ \omega_{hl}^H] = \begin{bmatrix} \frac{\partial Th_1^{\text{OUT}}}{\partial K_{111}^H} & \dots & \frac{\partial Th_1^{\text{OUT}}}{\partial K_{ijk}^H} \\ \vdots & \ddots & \vdots \\ \frac{\partial Th_i^{\text{OUT}}}{\partial K_{111}^H} & \dots & \frac{\partial Th_i^{\text{OUT}}}{\partial K_{ijk}^H} \\ \frac{\partial Tc_1^{\text{OUT}}}{\partial K_{111}^H} & \dots & \frac{\partial Tc_1^{\text{OUT}}}{\partial K_{ijk}^H} \\ \vdots & \ddots & \vdots \\ \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{111}^H} & \dots & \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{ijk}^H} \end{bmatrix} \quad (9)$$

$$[\omega_1^C \ \dots \ \omega_{cl}^C] = \begin{bmatrix} \frac{\partial Th_1^{\text{OUT}}}{\partial K_{111}^C} & \dots & \frac{\partial Th_1^{\text{OUT}}}{\partial K_{ijk}^C} \\ \vdots & \ddots & \vdots \\ \frac{\partial Th_i^{\text{OUT}}}{\partial K_{111}^C} & \dots & \frac{\partial Th_i^{\text{OUT}}}{\partial K_{ijk}^C} \\ \frac{\partial Tc_1^{\text{OUT}}}{\partial K_{111}^C} & \dots & \frac{\partial Tc_1^{\text{OUT}}}{\partial K_{ijk}^C} \\ \vdots & \ddots & \vdots \\ \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{111}^C} & \dots & \frac{\partial Tc_j^{\text{OUT}}}{\partial K_{ijk}^C} \end{bmatrix} \quad (10)$$

where a column stands for the sensitivity factors of a bypass to all the stream output temperatures.  $w_{i,hl}^H$  and  $w_{j,hl}^H$  are the elements of the sensitivity factor matrices regarding the bypasses in the hot sides of the heat exchangers, described as:  $w_{i,hl}^H = \partial Th_i^{\text{OUT}}/\partial K_{ijk}^H$  and  $w_{j,hl}^H = \partial Tc_j^{\text{OUT}}/\partial K_{ijk}^H$ .

To compare the sensitivity of each bypass to the entire HEN, the sensitivity factors of each bypass are classified by their average values. As described in Eqs. (11a)–(12b), the sensitivity factors are classified into the positive and negative ones with the same absolute value (1 and  $-1$  are used in this paper). Then, the number of positive and negative values determines the signs of the column summations in the classified matrix formed by the classified sensitivity factors. Such column summation is greater than 0 when the number of the positive values is greater than that of the negative values, as shown in Eqs. (13)–(14). Therefore, the bypass whose column summation is greater than zero is more sensitive to the entire HEN, which is described by Eqs. (15)–(16).

$$(-1)^{z_{i,hl}^{\text{eH}}} (p_{hl}^H - w_{i,hl}^H) \geq \delta z_{i,hl}^{\text{eH}} \quad (11a)$$

$$(-1)^{z_{j,hl}^{\text{eH}}} (p_{hl}^H - w_{j,hl}^H) \geq \delta z_{j,hl}^{\text{eH}} \quad (11b)$$

$$(-1)^{z_{i,cl}^{eC}} (p_{cl}^C - w_{j,cl}^C) \geq \delta z_{j,cl}^{eC} \quad (12a)$$

$$(-1)^{z_{i,cl}^{eC}} (p_{cl}^C - w_{i,cl}^C) \geq \delta z_{i,cl}^{eC} \quad (12b)$$

$$e_{hl}^H = \sum_i (-1)^{z_{i,hl}^{eH}} + \sum_j (-1)^{z_{j,hl}^{eH}} \quad (13)$$

$$e_{cl}^C = \sum_i (-1)^{z_{i,cl}^{eC}} + \sum_j (-1)^{z_{j,cl}^{eC}} \quad (14)$$

$$(\delta - (-1)^{z_{ijk}^{H,bys}}) e_{hl}^H \geq 0 \quad (15)$$

$$(\delta - (-1)^{z_{ijk}^{C,bys}}) e_{cl}^C \geq 0 \quad (16)$$

where  $p_{cl}^H$  and  $p_{cl}^C$  are the average values within the sensitivity factors of bypass to all the stream output temperatures. Binary variables  $z_{i,hl}^{eH}$ ,  $z_{j,hl}^{eH}$ ,  $z_{i,cl}^{eC}$  and  $z_{j,cl}^{eC}$  are proposed to examine the sign of each classified sensitivity factor.  $e_{hl}^H$  and  $e_{cl}^C$  are proposed to measure the column summations of the classified matrices for the bypasses in the hot and cold sides of the heat exchangers, respectively.  $\delta$  is a small positive constant. Binary variables  $z_{ijk}^{H,bys}$  and  $z_{ijk}^{C,bys}$  are proposed to denote the existence of all the promising bypasses to enforce binary variables  $z_{ijk}^{H,by}$  and  $z_{ijk}^{C,by}$  that are employed to describe the existence of the final selected bypasses:

$$z_{ijk}^{H,bys} - z_{ijk}^{H,by} \geq 0 \quad (17)$$

$$z_{ijk}^{C,bys} - z_{ijk}^{C,by} \geq 0 \quad (18)$$

### 3.4. Simultaneous synthesis of flexible and controllable HEN

The identification and quantification of disturbance propagations are employed to optimize the initial fractions of all the potential bypasses. And then the sensitivity factor is defined to determine the bypasses which are very sensitive to the entire HEN. In this way, the superstructure-based MINLP model for the synthesis of flexible and controllable HEN includes process models, the models with respect to the disturbance propagation identification and quantification, and sensitivity factor, and then additional models for bypasses.

Objective function: minimizing the total annual cost

$$\begin{aligned} \min & \left( \sum_i \sum_j \sum_k C z_{ijk} + \sum_i \sum_j \sum_k C^{HE} (A_{ijk})^\beta \right) \\ & + \left( \sum_i C z_i^{CU} + \sum_i C^{CU} (A_i^{CU})^\beta + \sum_i C^{CU} Q_i^{CU} \right) \\ & + \left( \sum_j C z_j^{HU} + \sum_j C^{HU} (A_j^{HU})^\beta + \sum_j C^{HU} Q_j^{HU} \right) \end{aligned} \quad (19)$$

where  $z_{ijk}$ ,  $z_j^{HU}$  and  $z_i^{CU}$  denote the existence of the heat exchangers, heaters and coolers, respectively.  $A_{ijk}$ ,  $A_j^{HU}$  and  $A_i^{CU}$  denote the areas of the heat exchangers, heaters and coolers, respectively. In Eq. (19), the first item means the costs of all heat exchangers, the second and third items mean the costs of coolers and heaters, respectively.

Constraints:

#### (a) Process models

All the process models are referred to Escobar *et al.* [10] and established by the non-split two-stage superstructure of HENs involving all the possible bypasses. For instance, the heat balance model for each stream is employed to ensure sufficient heating

or cooling so that the stream output temperatures reach its desired setting points at the end of the superstructure; the energy balance model is added to define the duty of the utilities, and the constraints of feasible temperature are employed to ensure the temperature decreases (hot streams) or increases (cold streams) along the stages. The process models are given in Appendix A and more details can also be found in the work of Escobar *et al.* [10].

#### (b) Models for the sensitivity factor, the disturbance propagation identification and quantification

This set of constraints can be seen in Eqs. (1)–(18).

#### (c) Additional models for bypasses

To denote the existence of the selected bypasses, binary variables  $z_{ijk}^{H,by}$  and  $z_{ijk}^{C,by}$  are also enforced by the differences between the inlet and output temperatures of the heat exchangers:

$$Th_{ijk}^{mix} - Th_{ijk}^{OUT,HE} \leq M z_{ijk}^{H,by} \quad (20)$$

$$Tc_{ijk}^{mix} - Tc_{ijk}^{OUT,HE} \geq -M z_{ijk}^{C,by} \quad (21)$$

where  $Th_{ijk}^{mix}$ ,  $Tc_{ijk}^{mix}$ ,  $Th_{ijk}^{OUT,HE}$  and  $Tc_{ijk}^{OUT,HE}$  are the temperature of the mixing junction and the output temperatures of a heat exchanger, respectively.  $M$  is a big positive constant. Eq. (20)/Eq. (21) implies that a bypass exists when the temperature difference of the bypassed exchanger is greater/smaller than zero.

Other logical constraints for bypasses are defined as:

$$z_{ijk}^{H,by} \leq z_{ijk}, \quad z_{ijk}^{C,by} \leq z_{ijk} \quad (22)$$

$$z_{ijk}^{H,by} - K_{ijk}^H \geq 0, \quad z_{ijk}^{C,by} - K_{ijk}^C \geq 0 \quad (23)$$

Eq. (22) represents that a bypass does not exist when the relevant binary variable  $z_{ijk}$  is equal to zero. Eq. (23) implies that the bypass fraction is equal to zero when this bypass does not exist. Then, the lower bound for the number of the selected bypasses is employed to avoid a negative degree of freedom, which is described as:

$$\sum_i \sum_j \sum_k (z_{ijk}^{H,by} + z_{ijk}^{C,by}) \geq i + j \quad (24)$$

## 4. Case Study

In this case, dynamic simulation and quantitative measures for flexibility and controllability are employed to illustrate the proposed method. Flexibility index is employed for the flexibility analysis of the obtained HEN, meanwhile, the controllability metrics are involved for the controllability analysis. By the dynamic simulation, the comparison of the dynamic behavior of the HENs can be used to further demonstrate the flexibility and controllability. It is noted that the main focus here is just to show that the design can be implemented in practice. Hence, additional improvements in the dynamic behavior made by different tuning controller parameters are not considered in this paper. The MINLP model is implemented in GAMS and solved using BARON [10]. This problem is performed on an Intel Core 3.6 GHz machine with 4 GB memory.

As listed in Table 1, the problem data is taken from the literature [5] and involves two hot streams and two cold streams.  $\Delta T_{min}$  is 10 K,  $U$  is 0.08 kW · m<sup>-2</sup> · K<sup>-1</sup> for all the matches. The costs of heating and cooling utilities are 147.4 USD · kW<sup>-1</sup> · a<sup>-1</sup> and 52.1 USD · kW<sup>-1</sup> · a<sup>-1</sup>, respectively. The ranges of variations for

**Table 1**  
Problem data for the case study

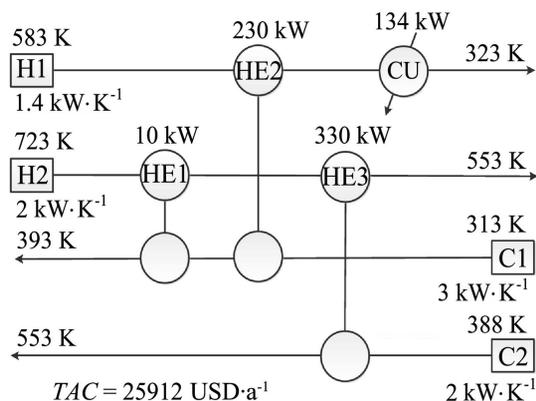
Stream	$T^N/K$	$T^{OUT}/K$	$F_{cp}/kW \cdot K^{-1}$
H1	583	323	1.4
H2	723	553	2.0
C1	313	393	3.0
C2	388	553	2.0
Hot utility	573	573	–
Cold utility	303	323	–

the expected disturbances are listed in Table 2, which is also taken from the literature [5].

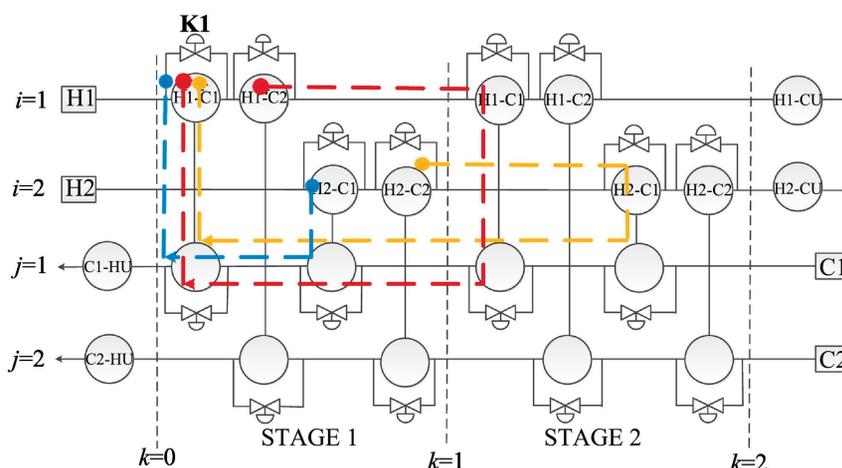
The initial HEN is obtained in nominal operating point, which is depicted in Fig. 4. The flexibility index is 0.13 calculated by the flexibility analysis method from the literature [25]. The result demonstrates that such HEN configuration is not flexible enough to withstand these expected disturbances. The literature intro-

**Table 2**  
Range of variations for disturbances

Uncertain parameter	Lower bound	Upper bound
$T_h^N/K$	573	593
$T_c^N/K$	383	393
$F_{cpH_1}/kW \cdot K^{-1}$	1.0	1.8
$F_{cpC_2}/kW \cdot K^{-1}$	1.6	2.4



**Fig. 4.** Optimal heat exchanger network configuration under the nominal condition.



**Fig. 5.** Possible disturbance loops for bypass K1.

duced the additional heat exchangers/heaters (coolers) and increased heat exchanger areas to improve the flexibility [5]. However, this may lead to a drastic increase of the total annual cost and then the further optimization has to be considered, such as area optimization. And when controllability is sequentially achieved, the potential difficulties in control designs may still arise.

To address these problems, this paper presents a method for simultaneously synthesizing flexible and controllable HEN. With this method, the disturbance propagations are identified and quantified to optimize the initial bypass fractions. As an example, the disturbance loops propagating from the potential heat exchangers in stage 1 to bypass K1 are shown in Fig. 5. Similarly, it is possible to give the disturbance loops propagating from other heat exchangers. The disturbance index of bypass K1 is determined through the existence of the heat exchangers in these disturbance loops. Then, the classified sensitivity factors of the potential bypasses to all the stream output temperatures are obtained. To facilitate analysis, two classified matrices are used to describe the classified sensitivity factors of the bypasses in the hot and cold sides of the heat exchangers, respectively, as shown in Eqs. (25)–(26).

$$W^H = \begin{bmatrix} -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 \end{bmatrix} \quad (25)$$

$$W^C = \begin{bmatrix} -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad (26)$$

The matrices include the rows of the stream output temperatures and the columns of all the possible bypasses with a total number of 16. The elements of the matrices are obtained by Eqs. (11a)–(12b). The sign of a column summation is employed to measure the sensitivity of a bypass to all the stream output temperatures. Then, the existence of the promising bypasses is described in the following matrices:

$$z^{H,bys} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad (27)$$

$$z^{C,bys} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad (28)$$

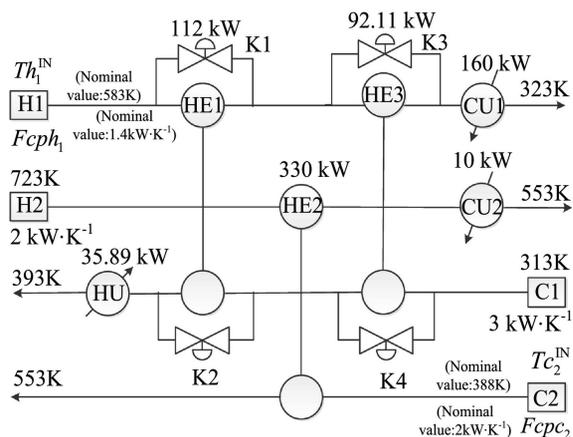


Fig. 6. Flexible and controllable heat exchanger network.

The matrices include the rows of the superstructure stages and the columns of the bypasses which are sequentially located in two stages. As shown in Eqs. (27)–(28), the number of the promising bypasses is greater than that of the streams. This implies that positive degree of freedom has been achieved. To facilitate analysis, the middle values of all the bypass fractions are assumed to be constant with 0.5. The bypasses are added in order to achieve the satisfactory flexibility and controllability, and new heat exchangers and the additional heat exchanger areas may also be considered. Then, a HEN design considering flexibility and controllability is obtained, which is depicted in Fig. 6. There exist 278 equations and 60 binary variables in the MINLP model for this case, and the computing time is acceptable with 964.0 s. The initial fractions of bypasses K1, K2, K3 and K4 are 0.01, 0.5, 0.5 and 0.5, respectively.

The total annual cost is 37404 USD·a<sup>-1</sup> with an 8.26% decrease to the result obtained by Li *et al.* [5]. The detailed comparison with the literature is shown in Table 3. In the literature, the increase of the heat exchanger area first was considered for improving HEN flexibility. In two heat exchangers, the ratios of the increased area were greater with 18.30% and 26.63%, respectively. In contrast, this paper adds the bypasses to explore the coupling between flexibility and controllability, subsequently, implementing their simultaneous consideration in HEN synthesis. The possible bypass fractions may introduce an increase in the utility consumptions. But comparing with the literature, the ratio of the increased operating cost in this paper does not significantly increase under the same numbers of the increased heaters/coolers. Further evidence is the increased costs comparing with the initial HENs. In the literature, the total annual cost for designing a flexible HEN was found with a 55.71% increase to that of its initial HEN. This paper gives a flexible and controllable HEN, whose cost is found with a 44.33% increase.

Furthermore, quantitative measures are given to analyze the flexibility and controllability of the obtained HEN. The flexibility analysis shows a satisfactory flexibility index of 1. The controllability of the HEN is analyzed by two controllability metrics: the condition number and the minimum singular value [10]. They are associated with the following logical statements: the saturation

problems should be avoided by minimum singular value closing to the largest possible; the condition number must be the lowest possible [10]. The control structure needs to be designed to calculate the above metrics.

Due to the combinatorial nature of the HENs, the control structure design problem below is based on the relative gain array (RGA) to find a control structure with minimum control loop interaction [26]. It is noted that a potential bypass on the hot side of heat exchanger HE2 may be selected to take control of the output temperature of stream H2/C2, as shown in Eqs. (27)–(28). And cooler CU2 and heater HU also may be employed for control purposes. In this way, control structure CS1 formed by the control loops ( $Th_1^{OUT}$  and  $K_{111}^C$ ;  $Th_2^{OUT}$  and  $Q_2^{CU}$ ,  $Tc_1^{OUT}$  and  $K_{112}^C$ ;  $Tc_2^{OUT}$  and  $K_{221}^H$ ) is finally obtained. Where bypass K5 (bypass fraction  $K_{221}^H$ ) is placed in the hot side of heat exchanger HE2 and added in the HEN for control purposes. The flexible and controllable HEN including this control structure is denoted in Fig. 7. A possible control structure CS2 formed by the control loops ( $Th_1^{OUT}$  and  $K_{111}^C$ ;  $Th_2^{OUT}$  and  $Q_2^{CU}$ ,  $Tc_1^{OUT}$  and  $K_{111}^H$ ;  $Tc_2^{OUT}$  and  $K_{221}^H$ ) is involved to compare. Evidently, control structure CS1 is superior to CS2 in terms of control loop interaction.

To compare with the results of controllability measures from the work of Escobar *et al.* [10], the flexibility of the obtained HEN needs to be measured again in the presence of the expected disturbances from this literature. The variation ranges of the disturbances which are expected in the inlet stream temperatures are assumed to be  $\pm 10$  K [10]. Then, the flexibility analysis shows a satisfactory flexibility index of 1. The results comparing with that obtained by this literature are listed in Table 4. Two control structures CS3 and CS4 from the literature are included in such comparison. It is possible to conclude that: 1) in terms of minimum singular value, control structure CS4 is the most promising and 2) in terms of condition number, control structure CS1 is the most promising. But control structure CS2 is also desirable in the above controllability metrics. The analyses imply that even without a desirable control structure, the proposed method enables the HEN to avoid the potential control difficulties so that the possibility of achieving good controllability is increased.

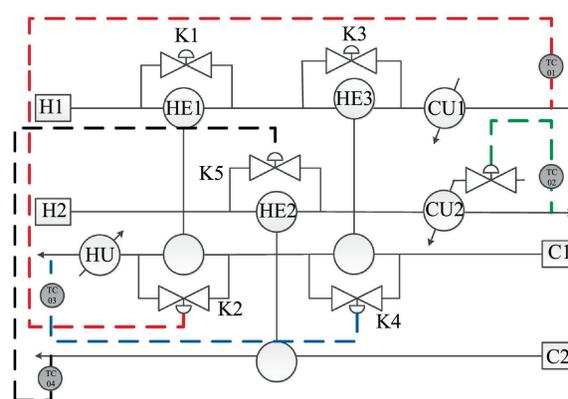


Fig. 7. The most promising control structure.

Table 3  
Comparison of the solution

Item	Operating cost/USD·a <sup>-1</sup>	Annual capital cost/USD·a <sup>-1</sup>	Total annual cost/USD·a <sup>-1</sup>	Number of heat exchangers
Li <i>et al.</i> [5]	11866	28626	40492	3
This work	14528	22876	37404	3

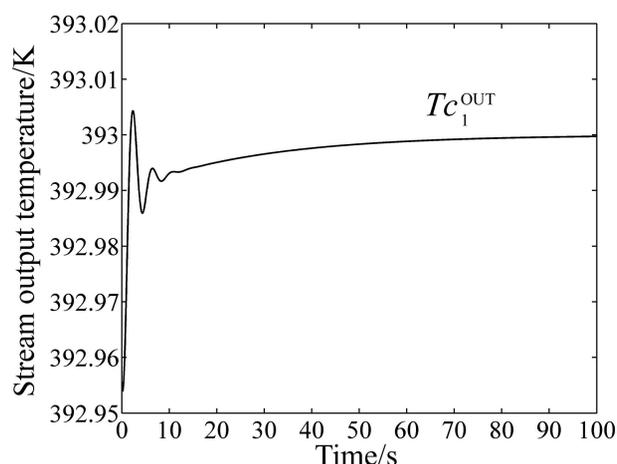
Table 4  
Controllability metrics evaluation for HENs with possible control structures

	This work		Escobar <i>et al.</i> [10]	
	CS1	CS2	CS3	CS4
Minimum singular value	0.16	0.11	0.44	2.33
Condition number	3.97	4.29	25.16	4.82

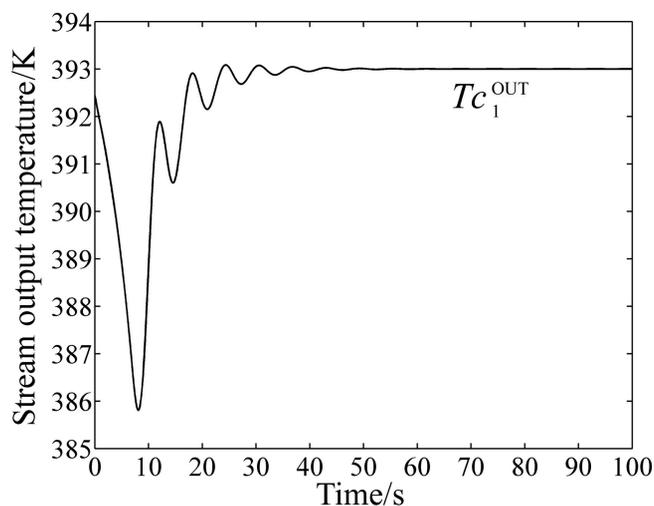
**Table 5**  
Control loop design with control structures CS1 and CS2

Control structure	Controlled variable	Manipulated variable	Setting point/K	Proportional gain	Integral time
CS1	$T_{C1}^{OUT}$	$K_{112}^C$	393	5.10	0.96
CS2	$T_{C1}^{OUT}$	$K_{111}^H$	393	-28.43	-0.89

On the other hand, the dynamic behavior of the HENs including control structures CS1 and CS2 respectively is analyzed to further demonstrate the flexibility and controllability. For the dynamic model see Appendix B for a brief derivation [10]. The comparison between the dynamic responses is employed to express the dynamic behavior. Such dynamic simulations are implemented in the MATLAB-Simulink environment. The change of setting point is +1 K assumed to happen in the output temperature of stream C1, meanwhile, the Proportional and Integral (PI) control strategy is involved. The specifications of the control loops are listed in Table 5, and the dynamic responses are shown in Figs. 8 and 9. For the output temperature of stream C1, the dynamic responses are specified in terms of rise time and maximum overshoot



**Fig. 8.** Dynamic response of output temperature of stream C1 within control structure CS1.



**Fig. 9.** Dynamic response of output temperature of stream C1 within control structure CS2.

allowed. The response of output temperature of stream C1 within control structure CS1 is smoother than that of control structure CS2. And the comparison in the rise times represents that bypass K4 (bypass fraction  $K_{112}^C$ ) can keep this temperature under regulation. As can be seen the HEN with control structure CS1 is able to reject the disturbances. But the regulation by bypass K1 (bypass fraction  $K_{111}^H$ ) still does not introduce negative effects on the dynamic behavior of the HEN. This implies that this HEN has the capability of withstanding the disturbances and increases the possibility of achieving the satisfactory controllability.

## 5. Conclusions

This work proposes a method for simultaneous synthesis of flexible and controllable HEN by considering their coupling. The key idea is to add bypasses to explore such coupling, and consequently ensuring feasibility and optimality of operation under the disturbances. A bypass is desirable with optimized initial fraction and position. For this purpose, the disturbance propagations from disturbance sources to sinks are identified and the numbers of the heat exchangers in the identified disturbance propagations are employed to quantify the disturbance propagations. These are both employed to optimize the initial fractions of all the potential bypasses. And then the sensitivity factors are defined to measure their sensitivity to the entire HEN so as to optimize the bypass positions. In this way, a HEN with optimized initial bypass fractions and bypass positions is obtained by solving a superstructure-based MINLP model. The proposed method is demonstrated through a case study: it gives a HEN with 8.26% lower total annual cost than that of the literature; the dynamic behavior, the flexibility index, the minimum singular value and the condition number show good flexibility and controllability of the obtained HEN. The results of the case study indicate that this method can efficiently address the simultaneous synthesis of flexible and controllable HEN. In presence of the disturbances, the HEN is guaranteed to operate without losing stream temperature targets while keeping an economically optimal energy integration.

## Nomenclature

$A_{ijk}$	Area for heat exchanger between hot stream $i$ , and cold stream $j$ , at stage $k$
$A_i^{CU}$	Area for heat exchanger between hot stream $i$ , and cold utility
$A_j^{HU}$	Area for heat exchanger between cold stream $j$ , and hot utility
$C^{A, CU}$	Area cost coefficient of coolers
$C^{A, HE}$	Area cost coefficient of heat exchangers
$C^{A, HU}$	Area cost coefficient of heaters
$C^F, CU$	Fixed charge of coolers
$C^F, HE$	Fixed charge of heat exchangers
$C^F, HU$	Fixed charge of heaters
$C^{M, CU}$	Fixed charge of cold utility cost per unit duty
$C^{M, HU}$	Fixed charge of hot utility cost per unit duty
$CL$	Set of bypasses in cold sides of heat exchangers
$e_{ci}^C$	A variable to measure column summations for bypasses on cold sides of heat exchangers
$e_{hi}^H$	A variable to measure column summations for bypasses on hot sides of heat exchangers
$F$	Set of heat exchangers
$F_{cp}C_j$	Heat capacity flowrate of cold stream $j$
$F_{cp}C_j^{HE}$	Heat capacity flowrate of potential bypassed cold stream $j$
$F_{cp}h_i$	Heat capacity flowrate of hot stream $i$
$F_{cp}h_i^{HE}$	Heat capacity flowrate of potential bypassed hot stream $i$
$HL$	Set of bypasses in hot sides of heat exchangers
$I$	Set of hot stream $i$

$J$	Set of cold stream $j$
$K_{ijk}^C$	Fraction of the bypass on the cold side of heat exchanger
$K_{ijk}^{C,md}$	Middle value of fraction of the bypass on the cold side of heat exchanger
$K_{ijk}^H$	Fraction of the bypass on the hot side of heat exchanger
$K_{ijk}^{H,md}$	Middle value of fraction of the bypass on the hot side of heat exchanger
$L$	Set of bypasses
$N_{l,s}$	Disturbance index of bypass $l$ in disturbance loop $s$
$O$	Set of heat exchangers in the same stream
$p_{cl}^C$	Average values within the sensitivity factors for bypasses on cold sides of heat exchangers
$p_{hl}^H$	Average values within the sensitivity factors for bypasses on hot sides of heat exchangers
$Q_i^{CU}$	Heat load between hot stream $i$ , and cold utility
$Q_{ijk}^{HE}$	Heat load between hot stream $i$ , and cold stream $j$ , at stage $k$
$Q_j^{HU}$	Heat load between hot stream $j$ , and hot utility
$Q_{Cj}$	Heat load of cold stream $j$
$Q_{Hi}$	Heat load of hot stream $i$
$S$	Set of disturbance loops
$ST$	Set of superstructure stages
$T_{Cj}^{IN}$	Inlet temperature of cold stream $j$
$T_{Cjk}^{IN,HE}$	Inlet temperature for heat exchanger between hot stream $i$ , and cold stream $j$ , at stage $k$
$T_{Cjk}^{mix}$	Temperature of the mixing junction of cold side in a heat exchanger
$T_{Cj}^{OUT}$	Output temperature of cold stream $j$
$T_{Cjk}^{OUT,HE}$	Output temperature for heat exchanger between hot stream $i$ , and cold stream $j$ , at stage $k$
$Th_i^{IN}$	Inlet temperature of hot stream $i$
$Th_{ijk}^{IN,HE}$	Inlet temperature for heat exchanger between hot stream $i$ , and cold stream $j$ , at stage $k$
$Th_{ijk}^{mix}$	Temperature of the mixing junction of hot side in a heat exchanger
$Th_i^{OUT}$	Output temperature of hot stream $i$
$Th_{ijk}^{OUT,HE}$	Output temperature for heat exchanger between hot stream $i$ , and cold stream $j$ , at stage $k$
$w_{i,cl}^C$	Elements of sensitivity factor matrix regarding the bypass in cold side of heat exchanger
$w_{j,cl}^C$	Elements of sensitivity factor matrix regarding the bypass in cold side of heat exchanger
$w_{i,hl}^H$	Elements of sensitivity factor matrix regarding the bypass in hot side of heat exchanger
$w_{j,hl}^H$	Elements of sensitivity factor matrix regarding the bypass in hot side of heat exchanger
$z_{ijk}$	Binary variable to existence of the match between hot stream $i$ , and cold stream $j$ , at stage $k$
$z_{ijk}^{C,s}$	Binary variable to existence of crucial heat exchanger in disturbance loop $s$
$z_{ijk}^{C,by}$	Binary variable to existence of the final selected bypasses in cold side of heat exchanger
$z_{ijk}^{C,bys}$	Binary variable to existence of the promising bypasses in cold side of heat exchanger
$z_i^{CU}$	Binary variable to existence of the match between hot stream $i$ , and cold utility
$z_{i,cl}^{eC}$	Binary variable to examine the sign of each classified sensitivity factors
$z_{j,cl}^{eC}$	Binary variable to examine the sign of each classified sensitivity factors
$z_{i,hl}^{eH}$	Binary variable to examine the sign of each classified sensitivity factors
$z_{j,hl}^{eH}$	Binary variable to examine the sign of each classified sensitivity factors
$z_{ijk}^{f,s}$	Binary variable to existence of first heat exchanger in disturbance loop $s$
$z_{ijk}^{H,by}$	Binary variable to existence of the final selected bypasses in hot side of heat exchanger

$z_{ijk}^{H,bys}$	Binary variable to existence of the promising bypasses in hot side of heat exchanger
$z_j^{HU}$	Binary variable to existence of the match between cold stream $j$ , and hot utility
$z_{ijk}^{H,s}$	Binary variable to existence of last heat exchanger in disturbance loop $s$
$z_{ijk}^{m,s}$	Binary variable to existence of middle heat exchanger in disturbance loop $s$

### Subscripts

$cl$	Bypass in cold side of heat exchanger
$hl$	Bypass in hot side of heat exchanger
$i$	Hot stream
$j$	Cold stream
$k$	Superstructure stage
$l$	Bypass
$s$	Disturbance loop

### Appendix A. Process Models for Synthesizing a HEN

(a) Heat balance for each heat exchanger:

$$Q_{ijk}^{HE} - Fcph_i^{HE} (Th_{ijk}^{IN,HE} - Th_{ijk}^{OUT,HE}) = 0 \quad (A1)$$

$$Q_{ijk}^{HE} - Fcpc_j^{HE} (Tc_{ijk}^{OUT,HE} - Tc_{ijk}^{IN,HE}) = 0 \quad (A2)$$

(b) Overall heat balance for each stream:

$$Fcp h_i (Th_i^{IN} - Th_i^{OUT}) = \sum_j \sum_k Q_{ijk}^{HE} + Q_i^{CU} \quad (A3)$$

$$Fcp c_j (Tc_j^{OUT} - Tc_j^{IN}) = \sum_i \sum_k Q_{ijk}^{HE} + Q_j^{HU} \quad (A4)$$

(c) Heat balance at each stage in superstructure:

$$Fcp h_i (Th_{i,k}^{st} - Th_{i,k+1}^{st}) = \sum_j Q_{ijk}^{HE} \quad (A5)$$

$$Fcp c_j (Tc_{j,k}^{st} - Tc_{j,k+1}^{st}) = \sum_i Q_{ijk}^{HE} \quad (A6)$$

(d) Non-isothermal streams mixing:

$$Th_{ijk}^{mix} = K_{ijk}^H Th_{ijk}^{IN,HE} + (1 - K_{ijk}^H) Th_{ijk}^{OUT,HE} \quad (A7)$$

$$Tc_{ijk}^{mix} = K_{ijk}^C Tc_{ijk}^{IN,HE} + (1 - K_{ijk}^C) Tc_{ijk}^{OUT,HE} \quad (A8)$$

(e) Flowrate balance for each heat exchanger:

$$Fcp h_i^{HE} = (1 - K_{ijk}^H) Fcp h_i \quad (A9)$$

$$Fcp c_j^{HE} = (1 - K_{ijk}^C) Fcp c_j \quad (A10)$$

(f) For logical constraints:

$$Q_{ijk}^{HE} - \Lambda_{ij} z_{ijk} \leq 0 \quad (A11)$$

$$Q_i^{CU} - \Lambda_i z_i^{CU} \leq 0 \quad (A12)$$

$$Q_j^{HU} - \Lambda_j z_j^{HU} \leq 0 \quad (A13)$$

(g) For approach temperatures:

$$dt_{ijk} \leq Th_{i,k}^{st} - Tc_{j,k}^{st} + \Gamma_{ij}(1 - z_{ijk}) \quad (A14)$$

$$dt_{ij,k+1} \leq Th_{i,k+1}^{st} - Tc_{j,k+1}^{st} + \Gamma_{ij}(1 - z_{ijk}) \quad (A15)$$

$$dt_i^{CU} \leq Th_{i,N_T+1}^{st} - Tc_{i,N_T+1}^{OUT} + \Gamma_{ij}(1 - z_{ijk}) \quad (A16)$$

$$dt_j^{HU} \leq Th_{j,1}^{OUT} - Tc_{j,1}^{st} + \Gamma_{ij}(1 - z_{ijk}) \quad (A17)$$

$$dt_{ijk}, dt_i^{CU}, dt_j^{HU} \geq \Delta T_{\min} \quad (A18)$$

(h) Assignment of inlet temperature in superstructure

$$Th_{i,0}^{st} = Th_i^{IN} \quad (A19)$$

$$Tc_{j,N_T+1}^{st} = Tc_j^{IN} \quad (A20)$$

(i) Feasibility constraints for temperatures

$$Th_{i,k}^{st} \geq Th_{i,k+1}^{st} \geq Th_i^{OUT} \quad (A21)$$

$$Tc_{j,k}^{st} \geq Tc_{j,k+1}^{st} \geq Tc_j^{IN} \quad (A22)$$

$$i \in I, j \in J, k \in ST$$

## Appendix B. Dynamic Modeling for a Given HEN

The dynamic models are based on the situation that there exist  $n$  heat exchangers in a HEN. They are referred to Escobar *et al.* [10], which can be described by the following equations:

$$\rho h V h_n cph \frac{dTh_n^{OUT,HE}}{dt} = mh cph (Th_{n-1}^{OUT,HE} - Th_n^{OUT,HE}) - U A_n \Delta T_n \quad (B1)$$

$$\rho c V c_n cpc \frac{dTc_n^{OUT,HE}}{dt} = mc cpc (Tc_n^{OUT,HE} - Tc_{n+1}^{OUT,HE}) - U A_n \Delta T_n \quad (B2)$$

$$\Delta T_n = \frac{(Th_{n-1}^{OUT,HE} - Tc_n^{OUT,HE}) + (Th_n^{OUT,HE} - Tc_{n+1}^{OUT,HE})}{2} \quad (B3)$$

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