Graph-theoretic Control Structure Synthesis for Optimal Operation of Heat Exchanger Networks

Lixia Kang and Yongzhong Liu

Abstract—In this paper, a recently developed procedure for the selection of control structure of heat exchanger networks for optimal operation is improved and reformulated in a graph-theoretic setting. A graph representing take-over relationship between the manipulations is constructed to generate the feasible split-range pairs based on active constraint regions. These feasible split-range pairs are then used to calculate a structural coupling matrix on the basis of the relative degree. The optimal control pairings are thus obtained through the solution of a bipartite matching problem, taking the structural coupling matrix as the weight matrix. A case study is used to verify the application of the proposed method.

I. INTRODUCTION

Large-scale chemical or petrochemical processes are highly energy intensive and usually require energy recovery systems to guarantee high efficiency of energy utilization and low cost of energy consumption [1]. Significant efforts have been focused on optimal operation of HENs [2]–[4], which is usually the framework of the nonlinear mathematical programming theory.

Alternative approaches dealing with the optimal operation problem usually involve real-time optimization and self-optimizing technologies, which turn out to be relatively expensive [5]. Some methods based on the structural information of HENs have also been developed for control structure selection, including analysis of input-to-output path in a cause and effect graph [6], the energy distribution routes in the network [7], and the sign of elements in transfer function matrix [8].

In fact, if there are no stream splits in HENs, the optimal operation of HENs can be modelled as linear programming, where the optimal solution is always at constraints [9]. In this direction, an offline optimization method was developed in [3]. However, in this method, a simplified relative degree was used as a measure of the interactions between the primary manipulations and controlled outputs. Thus, the interactions between the input/output pairs and those between the secondary input and the output are ignored. In addition, this simplification may fail to distinguish the effects of the bypass ratios around the hot and cold channels of the heat exchanger on the same controlled outputs. These simplifications may be one of the reasons for causing the multiple solutions in this problem.

A promising way to address this issue is to use the accurate relative degree as a measure of interactions between the inputs and outputs. It should be also noted that, for optimal input/output pairing problems, both the optimization-based and graph-based approaches have been developed on the basis of relative degree concept. In [10], relative degree was used to assess the dynamic effect of different manipulated inputs on economic cost functions in the context of economic model predictive control. Relative degree was also used as a measure of structural coupling to identify the optimal input/output pairs in [11]. It was further improved and reformulated in a graph-theoretic setting in [12] so that a decentralized control structure was obtained by solving a bipartite matching problem. Similar graph-theoretic formulism can also be found in [13]–[15]. The application of these methods is, somehow limited to the temperature control of HENs.

We should also note that the concept of graph theory has been extensively studied in the field of process synthesis and control. This was mainly done by adopting the graph decomposition technologies to minimize the communication cost [16] or interaction energy [17] in modern chemical and energy plants, electrical power systems, smart manufacturing systems, transportation networks and biological networks which typically feature a number of interacting subsystems [18]. Some process-based graphs (i.e. process flowsheet graph, P-graph, material/energy flow diagrams) have been employed for process synthesis [19], [20] or hierarchical control [21], [22]. Alternative graph representations on the basis of the process dynamics (i.e. cause and effect graph and equation graph) have also been used to generate control structure candidates [11], [23] or study some relevant problems [24] (i.e. structural controllability and observability).

To take advantage of these well-established graph-theoretic methods, an improved approach for control structure selection of HENs aiming at optimal operation is presented. The rest of the paper is organized as follows: a brief review of the graph-theoretic method for control structure selection is presented in section II where some terminology from graph theory are also provided. In section III, the graph-theoretic procedure for control structure selection of HENs aiming to minimize the utility costs is detailed. The application of the method is verified via a case study of a HEN in section IV and our conclusions are given in section V.

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II. GRAPH-THEORETIC METHOD FOR CONTROL STRUCTURE SELECTION

Consider a multiple-input and multiple-output nonlinear system determined by the equations:

\[ \dot{x} = f(x) + \sum_{i=1}^{n_u} g_i(x) u_i \]  
\[ y_j = h_j(x), \quad j = 1, 2, ..., n_y \]

where \( x \in \mathbb{R}^{n_x} \) is the state variable, and \( u_i, y_j \in \mathbb{R} \) denote the manipulated input and the controlled output, respectively. \( f \) and \( g_i \) are vector fields on \( \mathbb{R}^{n_x} \) while \( h_j \) is a scalar field on \( \mathbb{R}^{n_y} \). The relative degree of \( y_j \) with respect to \( u_i \), \( r_{ij} \), is defined as the smallest integer that satisfies [25]

\[ L g_i \left( L fight)_{(j)}^{-1} h_j(x) \neq 0 \]  
\[ \text{where } L \text{ represents the Lie derivative, defined as } \]
\[ L f h(x) = \frac{\partial h(x)}{\partial x} f(x) \]

It has been documented that the relative degree can be interpreted as a measure of how direct the effect of an input is on an output, and a measure of physical closeness between an input and an output [26]. Its calculation requires only structural information and can be automated on the equation graph that is a digraph where vertices represent the state, input and output variables, and edges are determined by mass and energy conservation equations on the basis of the following rules:

- there is an edge from node \( x_k \) to \( x_l \) if \( \frac{\partial f_k(x)}{\partial x_l} \neq 0 \);
- there is an edge from node \( u_i \) to \( x_l \) if \( \frac{\partial g_i(x)}{\partial x_l} \neq 0 \);
- there is an edge from node \( x_k \) to \( y_j \) if \( \frac{\partial h_j(x)}{\partial x_k} \neq 0 \),

where \( f_i(x) \) and \( g_{il}(x) \) are the \( l \)-th element of vector functions \( f(x) \) and \( g_l(x) \). In this digraph, a path is a sequence of distinct edges which connect a sequence of distinct vertices and are directed in the same direction. An input-to-output path \((u_i, y_j)-\text{path}\) is a path which starts from an input node and terminates at an output node. The length of a path, \( l \) is the number of edges included in the path. The relative degree, \( r_{ij} \) is then related to the length of the shortest input-to-output path connecting \( u_i \) and \( y_j \) of the digraph as follows [26]:

\[ r_{ij} = l_{ij} - 1 \]  

The relative degree matrix (RDM), \( R \) is thus formed, where the elements are the relative degrees between the inputs and the outputs.

\[ R = \begin{bmatrix} u_1 & \cdots & y_1 & \cdots & u_n \\ r_{11} & \cdots & r_{1n_y} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ u_{n_u} & \cdots & r_{n_u,1} & \cdots & y_n \end{bmatrix} \]

Taking the relative degree as a measure of the structural coupling in the network, a structural coupling criterion, \( s_{ij} \) was developed in [12], which is the sum of differences of the reversed relative degree, \( \bar{r}_{ij} \) from all the other reversed relative degrees associated with the input, \( u_i \), or the output \( y_j \),

\[ s_{ij} = \sum_{j'=1}^{n_y} (\bar{r}_{ij} - \bar{r}_{ij'}) + \sum_{i'=1}^{n_u} (\bar{r}_{i'j} - \bar{r}_{i'j'}) \]

\[ = (n_u + n_y) \bar{r}_{ij} - \sum_{i'=1}^{n_u} \bar{r}_{i'j} + \sum_{j'=1}^{n_y} \bar{r}_{ij'} \]  

Note that a larger value of \( s_{ij} \) means that the relative degree between \( u_i \) and \( y_j \), \( r_{ij} \) is less than most of the other relative degrees associated with the input \( u_i \) and the output \( y_j \), so that \( u_i/y_j \) is a favorable input/output pair to be selected. A structural coupling matrix, \( S_{U/Y} \) is then accordingly constructed. Note that, in \( S_{U/Y} \), \( s_{ij} \) will be reset to zero when it is calculated to be a negative value.

Taking the sets of the inputs, \( U \) and the outputs, \( Y \) as two vertex sets, \( S_{U/Y} \) as the weight matrix, a bipartite graph is constructed. The optimal input/output pairs of the network are then generated by finding a maximum weighted matching from this bipartite graph.

The procedure for selection of control structure can thus be summarized as follows:

- construct an equation graph according to the mass and energy balance equations;
- calculate the relative degree matrix, \( R \) by automated searching the shortest \( u_i, y_j \)-path in equation graph via Dijkstra's algorithm [27];
- establish the structural coupling matrix (SCM), \( S_{U/Y} \);
- identify the optimal input/output pairs through the solution of the bipartite matching problem, using Hungarian algorithm [27].

Note that the time complexities of the Dijkstra's algorithm and Hungarian algorithm are \( O(|V|^2) \) and \( O(|V|^3) \), respectively, where \( |V| \) stands for the number of the vertices in the corresponding graph. This implies that these graph-theoretic algorithms are efficient, scaling well with the size of the networks (or the number of the vertices).

This method has simply been used for temperature control of HENs. It will be extend to address the problem of optimal operation control of HENs in subsequent section.

III. GRAPH-THEORETIC CONTROL STRUCTURE SELECTION FOR OPTIMAL OPERATION OF HENS

In [3], the problem of control structure selection for optimal operation of the HEN was divided into two sub-problems: (1) identification of optimal split-range pairs for tracking active constraints during the operation, and (2) screening of appropriate control pairings for fast control action. These two sub-problems were simultaneously solved by an ILP with a weighted objective function. Note that one split-range pair contains only two manipulations.

In this section, we reformulate the problem of optimal operation of the HEN in a graph-theoretic setting, and solve it by using an improved procedure in the sense of structural coupling. Initially, a graph, representing the take-over relationship between the manipulations is constructed so that all potential manipulations and split-range pairs are generated.
By defining an improved structural coupling matrix on the basis of relative degree, the optimal control pairings are then selected through the solution of a bipartite matching problem. The primary and secondary manipulations are finally determined to finalize the synthesis of the control structure for optimal operation of the HEN.

A. Identification of feasible split-range pairs

For a set of given information about the disturbances, sets of active constraints regions can be obtained through parameter programming. The states of the manipulations, i.e. inactive, active on lower bound or upper bound, in each active constraint region can be uniquely determined. A graph, representing the take-over relationship between the manipulations can be formed according to the following rules:

- if a manipulated input is always an active constraint, it will be eliminated for not being used for manipulating purposes. Otherwise, each manipulated input will be represented as a single node in the graph.
- if a manipulated input is never an active constraint, it is represented as a node that has no connections with other nodes. The reason is that it should be only used for a primary manipulation that has no need of a secondary manipulation and is not used as a secondary manipulation.
- if a manipulated input changes between being an active constraint and an inactive one, and it is not active with the other one at the same region, there will be an edge between these two manipulations.

Note that, in this graph, each node is a feasible manipulation, and two nodes connected by an edge represent a feasible split-range pair. Thus, the number of edges is equal to the feasible split-range pairs in the HEN. We thus define the set of feasible manipulations, \( U \), whose elements are these feasible split-range pairs and the manipulations represented as an isolated node in the graph.

B. Selection of optimal control pairings

To consider the interactions between the input/output pairs as well as those between the secondary inputs and the corresponding outputs, an improved SCM, \( S_{U/Y} \) is constructed, whose element, \( s_{ij} \), is expressed as:

\[
s_{ij} = s_{ij} + s_{i'j}
\]

where the subscripts \( i \) and \( i' \) stand for the manipulated inputs, \( u_i \) and \( u_{i'} \) in a feasible split-range pair, and \( j \) is the corresponding controlled output, \( y_j \), and \( s_{ij} \) and \( s_{i'j} \) are the \((i,j)^{th}\) and \((i',j)^{th}\) elements in \( S_{U/Y} \), respectively.

Likewise, a bipartite graph, taking \( S_{U/Y} \) as the weight matrix is constructed. The optimal control pairings are then obtained by solving a maximum weighted matching problem. The output of this problem is a \( n_y \times n_y \) matrix, \( P_{opt} \), whose element is 1 if the control pairing is selected, and 0 otherwise.

Now we are in the position to determine the primary and secondary manipulations in split-range pairs by the following rules:

- if an input appears in more than two selected split-range pairs, it will be considered a secondary manipulated input.
- if an input appears in only one selected split-range pairs and has a smaller relative degree associated with the corresponding controlled output, it will be selected the primary manipulated input in this split-range pair.

The proposed procedure for control structure selection of the HEN aiming at optimal operation is thus summarized as follows:

- calculate the RDM, \( R \) based on equation graph
- construct the SCM, \( S_{U/Y} \)
- generate the feasible split-range pairs
- calculate the improved SCM, \( S_{U/Y}^{'} \)
- identify the optimal control pairings via bipartite matching

IV. CASE STUDY

In this section, a HEN with two hot streams and two cold streams is used to illustrate the application of the proposed method, as shown in Fig. 1. This example comes from [3] where only the single bypass and the flowrate of utility are considered as the manipulated inputs. We define the following set of the manipulated inputs, \( U \) and the set of the controlled outputs, \( Y \)

\[
U = \{ Q_{c1}, Q_{c2}, Q_{h1}, u_{b1}, u_{b2}, u_{b3} \} \\
Y = \{ T_3, T_5, T_8, T_9 \}
\]

A. Control structure selection for temperature control of HEN

The mass and energy balances of the HEN is given as:

\[
\frac{dT_1}{dt} = \frac{F_{h1}(T_{h1}^{in} - T_1)}{V_1} - \frac{u_{b1}UA_1}{\rho Cp V_1} \Delta T_{L,1} 
\]

\[
\frac{dT_2}{dt} = \frac{F_{h1}(T_1 - T_2)}{V_2} - \frac{U_{A2}}{\rho Cp V_2} \Delta T_{L,2} 
\]

\[
\frac{dT_3}{dt} = \frac{F_{h1}(T_2 - T_3)}{V_1} - \frac{Q_{c1}}{\rho Cp V_1} 
\]

\[
\frac{dT_4}{dt} = \frac{F_{h2}(T_{h2}^{in} - T_4)}{V_3} - \frac{u_{b2}UA_2}{\rho Cp V_3} \Delta T_{L,3} 
\]
\[
\begin{align*}
\frac{dT_5}{dt} &= \frac{F_{h2}(T_4 - T_5)}{V_{c2}} - \frac{Q_{c2}}{\rho C_p V_{c2}} \\
\frac{dT_6}{dt} &= \frac{F_{c1}(T_{in} - T_6)}{V_1} + \frac{U A_1}{\rho C_p V_1} \Delta T_{L,1} \\
\frac{dT_7}{dt} &= \frac{F_{c1}(T_7 - T_7)}{V_3} + \frac{U A_3}{\rho C_p V_3} \Delta T_{L,3} \\
\frac{dT_8}{dt} &= \frac{F_{c1}(T_8 - T_8)}{V_h} + \frac{Q_b}{\rho C_p V_h} \\
\frac{dT_9}{dt} &= \frac{F_{c2}(T_{in} - T_9)}{V_2} + \frac{u_{u2}U/A_2}{\rho C_p V_2} \Delta T_{L,2}
\end{align*}
\]

where \(T\) is the temperature, \(Q\) and \(F\) stand for the utility heat load and the volumetric flow rate of the streams. \(U A\) is the product of overall heat transfer coefficient and the heat transfer area. \(V\) is the volume of the unit while \(\rho\) and \(C_p\) are the density and specific heat capacity of streams, respectively. \(\Delta T_L\) is the logarithmic mean temperature difference of heat exchanger.

According to eqs. (8)-(16), an equation graph, representing the structural relationship between the variables is constructed in Fig. 2. The RDM, \(R\) and the corresponding structural coupling matrix, \(S_{U/Y}\) are calculated as

\[
R = \begin{bmatrix}
T_3 & T_5 & T_8 & T_9 \\
Q_{c1} & 1 & \infty & \infty & \infty \\
Q_{c2} & \infty & 1 & \infty & \infty \\
Q_{b1} & \infty & \infty & 1 & \infty \\
u_{u1} & 3 & 4 & 3 & 2 \\
u_{u2} & 2 & \infty & \infty & 1 \\
u_{u3} & \infty & 2 & 2 & \infty
\end{bmatrix}
\]

\[
S_{U/Y} = \begin{bmatrix}
Q_{c1} & T_3 & T_5 & T_8 & T_9 \\
Q_{c2} & 0 & 7.25 & 0 & 0 \\
Q_{b1} & 0 & 0 & 7.167 & 0 \\
u_{u1} & 0.083 & 0 & 0.083 & 2.083 \\
u_{u2} & 1.667 & 0 & 0 & 7 \\
u_{u3} & 0 & 2.25 & 2.167 & 0
\end{bmatrix}
\]

Taking \(S_{U/Y}\) as the weight matrix, a bipartite graph is then constructed, and the optimal input/output pairs, \((Z_{opt})\) are thus returned through the solution of the maximum weighted matching problem, i.e.

\[
Z_{opt} = \begin{bmatrix}
Q_{c1} & 1 & 0 & 0 & 0 \\
Q_{c2} & 0 & 1 & 0 & 0 \\
Q_{b1} & 0 & 0 & 1 & 0 \\
u_{u1} & 0 & 0 & 0 & 1
\end{bmatrix}
\]

The optimal RDM, \(R_{opt}\) is then obtained \((R_{opt} = Z_{opt}R)\).

\[
R_{opt} = \begin{bmatrix}
Q_{c1} & 1 & \infty & \infty & \infty \\
Q_{c2} & \infty & 1 & \infty & \infty \\
Q_{b1} & \infty & \infty & 1 & \infty \\
u_{u2} & 2 & \infty & \infty & 1
\end{bmatrix}
\]

Note that, for each row, the diagonal element has the smallest value, implying that each input is paired with the output that has the most direct effect on. In this configuration, the outlet temperatures of the cold streams \(C1\) and \(C2\) are controlled by manipulating the flow rates of the cooling utilities, and the outlet temperature of hot stream \(H1\) is controlled by manipulating the flow rate of the heating utility. The bypass ratio around the cold channel of HE2, \(u_{u2}\) is manipulated to control the outlet temperature of \(C2\). It also worthy noting that this assignment is consistent with previous guidelines for control of the HENs [2], [28].

**B. Control structure selection for optimal operation of HEN**

In [3], the disturbances were assumed the inlet temperature of each stream, with the expected variation \(\pm 10^\circ C\) for streams \(H1\), \(H2\), and \(C1\) and \(\pm 5^\circ C\) for stream \(C2\). This results in feasible LP optimal solutions and five active constraint regions using parametric programming, as given in Table 1.

**TABLE I: Sets of active constraints regions**

<table>
<thead>
<tr>
<th>Regions</th>
<th>(Q_{c1})</th>
<th>(Q_{c2})</th>
<th>(Q_{b1})</th>
<th>(u_{u1})</th>
<th>(u_{u2})</th>
<th>(u_{u3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>L</td>
<td>/</td>
<td>L</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>L</td>
<td>/</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>3</td>
<td>/</td>
<td>L</td>
<td>L</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>4</td>
<td>/</td>
<td>/</td>
<td>L</td>
<td>L</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>5</td>
<td>/</td>
<td>/</td>
<td>/</td>
<td>L</td>
<td>/</td>
<td>U</td>
</tr>
</tbody>
</table>

In this table, L and U stand for the saturated manipu-
lations (active constraints) at the lower and upper bounds, respectively and "/'" stands for the unsaturated manipulation (inactive constraint). It can be seen that \( Q_{c1}, Q_{c2} \) and \( Q_{h1} \) will become active at their lower bounds, implying the situation where the flow rates of the utilities are zero or the valves on the utility streams are fully closed. \( u_{b2} \) will become active at its upper bound, indicating that the valve on the bypass is fully open. Note that only one saturation is allowed for each manipulation.

\[
P_{opt} = \begin{bmatrix}
Q_{c1} - u_{b1} \\
Q_{c2} - u_{b3} \\
Q_{c2} - Q_{h1} \\
u_{b2}
\end{bmatrix}
\begin{bmatrix}
T_1 & T_5 & T_8 & T_9
\end{bmatrix}
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

This result indicates that the outlet temperature of stream H1 is controlled using a split-range scheme with the flow rate of cooling utility, \( Q_{c1} \) and the bypass ratio around the hot channel of HE1, \( u_{b1} \) as input pairs, and the outlet temperature of stream H2 is controlled using a split-range scheme with the flow rate of cooling utility \( Q_{c2} \) and the bypass ratio around the hot channel of HE3, \( u_{b3} \) as inputs. \( Q_{c2} \) and \( Q_{h1} \) are used as the split-range pairs to control the outlet temperature of stream C1 while the bypass ratio \( u_{b2} \) is manipulated to control the target temperature of stream C2.

The control pairing arrangement is summarized in Table 2. Note that in this arrangement, \( Q_{c2} \) will be used as a secondary manipulation because it appears in two split-range pairs. For split-range pair of \( Q_{c1} - u_{b1} \), \( Q_{c1} \) is selected as the primary manipulation because (1) it has more direct effect on the controlled output, \( T_3 \) according to \( R \) and (2) the input/output pair, \( Q_{c1}/T_3 \) is less affected by other control pairings than \( u_{b1}/T_3 \) according to \( S_{U/Y} \).

The control structure of the HEN for optimal operation is given in Figure 4. Note that these choices satisfy the optimization objectives in [3], but will, of course, need to be evaluated via simulations.

![Graph for control structure](image)

**Fig. 3: The take-over relationship between manipulations**

According to the rules presented in previous section, a graph, representing the take-over relationship between the manipulations is constructed, as shown in Fig. 3. Note that \( u_{b2} \) is represented as a single node without any connections with other nodes because it is unsaturated in all active constraint regions, implying that it will only be used for a primary manipulation that has no need of a secondary manipulation and is not used as a secondary manipulation. Fig. 3 also shows that there are five potential split-range pairs in this HEN. The elements in the set of potential manipulations, \( \mathcal{U} \) are the potential split-range pairs of \( Q_{c1} - u_{b1}, Q_{c1} - u_{b3}, Q_{c2} - Q_{h1}, Q_{c2} - u_{b3} \) and \( u_{b1} - u_{b3} \), as well as a manipulation, \( u_{b2} \).

Based on \( \mathcal{U} \) and \( S_{U/Y} \), an improved SCM, \( S'_{U/Y} \) associated with the potential manipulations and controlled outputs is calculated. Analogous to the procedure for control structure selection for temperature control of the HEN, a bipartite graph \( G'(\mathcal{U}, Y, S'_{U/Y}) \) is constructed and solved to generate the optimal control pairings as follows:

| \begin{bmatrix} T_5 & T_8 & T_9 \end{bmatrix} | \begin{bmatrix} T_3 & Q_{c1} & S_{b1} \end{bmatrix} |
|---|---|---|
| split-range control | 7.25 & 0 & 0.083 & 2.083 |
| split-range control | 7.167 & 2.25 & 2.167 & 0 |
| split-range control | 0 & 7.25 & 7.167 & 0 |
| split-range control | 0 & 9.5 & 2.167 & 0 |
| bypass control | 0.083 & 2.25 & 2.25 & 2.083 |
| bypass control | 3.334 & 0 & 0 & 14 |

**TABLE II: Final control pairing arrangement**

![Control structure diagram](image)

**Fig. 4: Control structure for optimal operation of HEN**

**V. CONCLUSIONS**

This paper addresses a graph-theoretic approach for synthesis of control structure for optimal operation of HENs.
The method is reformulated from a recently developed procedure, and it is improved by using a structural coupling criterion (based on the accurate relative degrees) to screen the control pairings instead of employing a simplified relative order. The method takes the advantage of the well-established graph theory algorithms, which facilitates the solution generation. In addition, the resulting control structure of the HEN satisfies the optimization objectives in literature so that the effectiveness of the method is verified.

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