DEVELOPMENT OF CONTROL STRUCTURE DESIGN AND STRUCTURAL CONTROLLABILITY FOR HEAT EXCHANGER NETWORKS

INTRODUCTION

Although a number of researches on heat exchanger networks (HENs) have been published since the last two decades, there is not much work on the control of HENs. This is the main motivation for this thesis. Two main issues on the control of HENs will be addressed here. The first issue concerns optimal operation of HENs, whereas the second issue concerns controllability improvement in HEN synthesis.

1. Motivation on optimal operation of heat exchanger networks

The increase in energy price motivates a need for heat recovery in a plant. Heat recovery can be obtained by integrating heat among some hot streams that need to be cooled and some cold streams that need to be heated, with the use of heat exchangers combined as heat exchanger networks in the plant. However, to achieve the reduction of energy cost in practice, an optimal operation strategy may be needed. In general, the term “optimal operation of HENs” requires that 1) target temperatures can be satisfied and 2) utility cost is minimized.

This work focuses on simple ways of implementing (economic) optimal operation of HENs. In general, we first control the active constraints, and for the remaining unconstraints we look for good ‘self-optimizing’ variables (Skogestad, 2000). For some problems, including the HEN problem considered in this work, there are no optimally unconstrained degrees of freedom, that is, all degrees of freedom should be used to satisfy active constraints. The issue in terms of implementing optimal operation is then to identify the active constraints and change the control policy accordingly. A naive (or at least rather complex) approach is to use on-line optimization. In this thesis, the approach is to use off-line optimization to identify all possible regions with different sets of active constraints and then attempt to find a simple operation policy for switching between regions. The approach taken here is to use split-range control, which probably is the simplest way of dealing with changes in active input constraints. Two approaches for the design of optimal split-range control structure will be proposed. The first approach is based on the information of directional effect among manipulated variables and controlled variables, whereas the second approach is based on the information of active constraint regions in a given disturbance window.

2. Motivation on HENs synthesis with controllability improvement

In general, the design methods of HENs are usually considered based on an economic objective. Unfortunately, the integration of streams in HENs may give an inherent control problem. Hence, the issue of controllability should be undertaken during the process design stage. This part of the research focuses on controllability of HENs. However, the term ‘controllability’ in this work will be limited to structural controllability in which only the physical relationship among inputs and outputs in the process is considered. To obtain HENs with well structural controllability, two ideas are proposed.

The first idea is the selection of the best solution among the solution set of HEN structure alternatives obtained from a number of synthesis techniques. In general, HEN synthesis techniques may provide more than one promising solution. Hence, to select the best one, a controllability evaluation may be needed. The structural analysis criteria based on structural singularities, right half plane zeros, time delays, and interactions will be implemented. The evaluation is formulated as an integer linear program.

The second idea is to look for a HEN structure solution with a number of subnetworks. The term ‘subnetworks’ means small independent HENs combined in a large HEN. One of the advantages of having several subnetworks is that operability and controllability problems are easier to manage since the system has less interaction

(Shethna and Jezowski, 2006). In this thesis, the MINLP HEN synthesis model of Yee and Grossman (1990) is modified by introducing additional binary variables and corresponding constraints to enforce the solutions to have at least user-specified number of subnetworks.

OBJECTIVES

1. To develop methodologies for control structure design to implement optimal operation of HENs

2. To develop methodologies to improve structural controllability in HEN synthesis stages

Scope of work

1. Develop methodologies for optimal split-range control structure design to implement optimal operation of special HENs that only single bypasses and utility duties are considered as manipulated variables.
2. Develop a structural controllability evaluation technique for HENs.
3. Modify the MINLP HEN synthesis model of Yee and Grossman (1990) for having solutions with a number of subnetworks.

LITERATURE REVIEW

Part I: Optimal operation of heat exchanger networks

To operate the plant in an optimal manner, one should first answer the two questions: (Q1) are there enough degrees of freedom (DOFs, or manipulated variables) for control? and (Q2) are there extra degrees of freedom for an optimization? The question (Q1) is used to check the possibility to control each controlled variable independently, while the question (Q2) is used to check whether except the control design for setpoint satisfaction, we also need to consider the economic objective or not. For heat exchanger networks, Marselle *et al.* (1982) proposed the definition of the number of degrees of freedom (N_{DOF}) by

$$N_{DOF} = N_{units} - N_t \qquad (1)$$

where N_{units} is the number of exchanger units or manipulated variables (degrees of freedom) and N_t is the number of target temperatures.

The condition $N_{DOF} > 0$ is necessary for the operation to be feasible and utility cost optimizable. However, this is not enough to answer the questions (Q1) and (Q2). The more precise definition of the number of degrees of freedom with respect to utility cost optimization ($N_{DOF,U}$) that was sufficient to answer the two questions was proposed by Glemmestad (1997) as shown in the following:

$$N_{DOF,U} = DS + N_U - N_t \qquad (2)$$

where DS is the dimensional space spanned by the manipulated variables in the inner HEN to the outer HEN and N_U is the number of utility types.

The implication of $N_{DOF,U}$ can be summarized as shown in Table 1. The operation will be structurally feasible (question Q1) if and only if the condition

$N_{DOF,U} \geq 0$ can be satisfied. Furthermore, there will be extra degrees of freedom for utility cost optimization (question Q2) if and only if $N_{DOF,U} > 0$.

Table 1 The implication of $N_{DOF,U}$

Case	**(Q1)**	**(Q2)**
$N_{DOF,U}<0$	No	No
$N_{DOF,U}=0$	Yes	No
$N_{DOF,U}>0$	Yes	Yes

It is obvious that the operation of HENs will be more challenging when $N_{DOF,U} > 0$ because aside from the setpoint satisfaction, the utility cost should also be minimized. This means that a common heuristic rule for the control design such as manipulating the last heat exchanger on a stream for a direct effect (Marselle *et al.*, 1982; Calandranis and Stephanopoulos, 1988; Mathisen, 1994) may not be preferred from an energy point of view.

Several strategies were proposed to handle optimal operation of HENs. The early researches were techniques based on structural information. Marselle *et al.* (1982) applied a graph theory to suggest a control structure and developed a control policy to adjust flow distributions in HENs to meet target temperatures with minimum utility usage. Calandranis and Stephanopoulos (1988) used the structural characteristics of HENs to identify routes to allocate loads to available sinks and developed a knowledge-based concept to select the best route. The methods based on structural information using a sign matrix (directional effect among manipulated variables and controlled variables) were proposed by Mathisen (1994) and Glemmestad *et al.* (1996).

However, the control design based on structural information cannot guarantee the optimality in some cases, such as when HENs contain heat load loops, hence a conventional online-optimization may be recommended. The researches based on online and periodic optimizations for optimal operation of HENs can be found in

Aguilera and Marchetti (1998), Glemmestad *et al.* (1999) and González *et al.* (2006). Nevertheless, online-optimization requires a rather complex approach for the implementation. Hence, some recent researches for the optimal operation have been devoted to simple ways of implementing (economic) optimal operation. For example, Skogestad (2000) proposed a concept of 'self-optimizing control', that is, finding a magic variable to keep constant and then resulting in optimality. Pistikopoulos *et al.* (2002) used offline parametric optimization to simplify the task of online optimization. This resulted in (a) no optimization solver is called on-line, and (b) only simple function evaluations are required.

This research proposes a new simple technique to implement optimal operation of HENs. For certain HENs that only single bypasses and utility duties are considered as manipulated variables, optimal operation of HENs can be formulated as a linear programming (LP) problem. The LP formulation implies that optimal solutions will always lie at some input constraint vertices. However, under the change of operating condition, the optimal vertex may change and this motivates a need of an idea for optimal switching between active constraints region. The implementation in this work is to use split-range control that is probably the easiest way to implement the switching. Two approaches to determine optimal split-range control structure are proposed. The first approach is based on directional effects among manipulated variables and control variables. The second approach is based on the information of active constraints that can be obtained from solving an offline optimization.

Part II: HENs synthesis with controllability improvement

The analysis of controllability during the process design has been criticized by many experts. Shinskey (1982) noted that "the plant may be uncontrollable even though the process design appears satisfactory from a steady-state point of view". Morari (1992) pointed out that some simple controllability criteria should be included within synthesis procedures and trade-off controllability and economic objectives. Skogestad and Postlethwaite (2005) stated that "Controllability is independent of the controller, and is a property of the plant (or process) alone. It can only be affected by changing the plant itself; that is, by (plant) design changes".

In general, integration techniques for process design and control can be categorized into two approaches: sequential and simultaneous approaches. In the first approach, design and control objectives will be considered step-by-step in a preference order, that is, after satisfying the first objective, the second objective will be considered, and so on. The advantage of this approach is that a large complicated problem can be decomposed into a number of small and less-complicated sub-problems. However, the solutions may be sub-optimal. In the latter approach, all design objectives are considered simultaneously and hence the trade-off among design and control objectives can be provided. However, this approach usually results in a big complicated problem and may be difficult to solve. Hence, the problem size seems to be limited.

Mathisen (1994) studied the effects of structural singularities, right half plane zeros, time delays, input constraints, and interactions on HENs. Several heuristics for the controllability improvement in HEN design were also proposed in this work. Westphalen *et al.* (2003) proposed condition number as a criterion for controllability analysis. The best condition number obtained from the alternative sets of manipulated variables is defined as controllability index of HENs. Furthermore, for HENs with subnetworks, controllability index is defined as the smallest value obtained from the set of the best condition number of each subnetwork. Tellez *et al.* (2006) proposed a five-step procedure with the use of several analysis tools to determine controllability of HENs and its potential control structure. Non-square relative gain array is first used for selecting appropriate control pairing and then controllability of the potential pairing is evaluated using condition number, performance relative gain array, disturbance condition number, closed-loop disturbance gain, partial disturbance gain, input constraint, and resiliency index. The techniques in the literatures above can be applied in the sequential approach for integrating design and control of HENs.

For the simultaneous approach to improve controllability of HENs, one possible technique is to include some heuristics into the synthesis model. The translation of some heuristics, such as avoiding double output matches, avoiding inner matches, avoiding parallel heat exchangers, etc., into constraint equations can be found in Mathisen (1994). Another attempt to include dynamic controllability into HEN synthesis was proposed by Papalexandri and Pistikopoulos (1994a and 1994b). Some simple controllability criteria was proposed and used to explore potential control structures simultaneously in the model. However, this resulted in a very complex model and hence the problem size seems to be limited.

Another technique that may be considered as a design for controllability improvement is to find out the solution of HENs with a number of subnetworks. Shethna and Jezowski (2006) showed the importance of having a number of subnetworks, that is: 1) total number of heat exchangers can be reduced; 2) operability and controllability problems are easier to manage; and 3) detailed design stage is easier. However, their objective was to find a maximum number of subnetworks in which the trade-off between investment (number of units and area) and utility costs was not considered.

This part of the research looks for a HEN synthesis method with focus on controllability improvement. Two methods to improve controllability in HEN synthesis are proposed. The first method concerns the sequential approach. The idea is that among the economically reasonable solution set, the solution with best controllability properties is preferred. However, only structural controllability properties are considered here. Structural controllability analysis requires only the physical relationship among inputs and outputs, hence it is possible to be applied in the beginning of a process design where the numerical information is limited (Srinophakun, 1996). A decentralized control is assumed. Structural analysis tools used are based on structural singularities, number of parallel opposing effects, relative orders (Daoutidis and Kravaris, 1992), and decoupling indices (Lee *et al.*, 2001) in which the evaluation is formulated as an integer linear program (ILP).

The second method concerns the simultaneous approach. The idea is that among the economically reasonable solution set, the solution with the more number of subnetworks is preferred. The MINLP HEN synthesis model of Yee and Grossman (1990) is modified by introducing additional binary variables and corresponding constraints to enforce the solution to have at least user-specified number of subnetworks.

MATERIALS AND METHODS

The hardware used in this work is Laptop AMD Turion64 MT30 with RAM 512 MB. The softwares used are: Aspen plus v12.1, Aspen dynamics v12.1, GAMS Build VIS 20.7 133, and MATLAB v7.

Part I: Optimal operation of heat exchanger networks

This part will describe the overall idea of implementing optimal operation of HENs in this thesis.

1. LP formulation for optimal operation of HENs

Consider heat exchanger networks where the objective is to maintain optimal operation in spite of the variations in the inlet temperatures. Assume:

a) Constant heat capacity flowrate (mC_P) for all streams
b) Constant heat transfer coefficients (UA) for all heat exchangers

Further assume that the available degrees of freedom for control (operation) are:

a) Single bypasses (duties of individual exchangers, Q)
b) Utility duties (Q_h, Q_c)

Under these assumptions, Aguilera and Marchetti (1998) showed that the corresponding steady-state optimal operation of HENs can be formulated as a linear programming (LP) problem:

$$\min \ c^T x$$

Subject to: (3)

$$Ax \leq b$$
$$A_{eq} x = b_{eq}$$
$$x_{\min} \leq x \leq x_{\max}$$

The vector *x* consists of the inlet and outlet temperatures on the hot side ($T_i^{hot,in}$ and $T_i^{hot,out}$) and cold side ($T_i^{cold,in}$ and $T_i^{cold,out}$) of all exchangers, as well as the duties of all exchangers (Q_i-process exchanger, Q_{ci}-cold utility exchanger and Q_{hi}-hot utility exchangers). The equality constraints include the process models, the internal connections, and given supply temperatures T_i^s and target temperatures T_i^t. The inequality constraints include the lower and upper bounds on the duties of all heat exchangers. The objective function allows for many problem formulations including maximum temperature problem. In this research, the objective is to minimize the utility cost in which all elements of the cost vector *c* are zero except the elements related to the duties of utility exchangers. The LP problem formulation for optimal operation of HENs is given in equations 4a-4m:

Objective function: $$\min \sum_{i \in CU} Ccu_i Q_{ci} + \sum_{j \in HU} Chu_j Q_{hj} \qquad (4a)$$

subject to

a) Process models (energy balances)

for process exchanger *i*:

$$Q_i - (mC_P)_i^{cold}\left(T_i^{cold,out} - T_i^{cold,in}\right) = 0 \qquad i \in PHX \qquad (4b)$$

$$Q_i - (mC_P)_i^{hot}\left(T_i^{hot,in} - T_i^{hot,out}\right) = 0 \qquad i \in PHX \qquad (4c)$$

for cooler i:

$$Q_{ci} - (mC_P)_i^{hot}\left(T_i^{hot,in} - T_i^{hot,out}\right) = 0 \qquad i \in CU \qquad (4d)$$

for heater i:

$$Q_{hi} - (mC_P)_i^{cold}\left(T_i^{cold,out} - T_i^{cold,in}\right) = 0 \qquad i \in HU \qquad (4e)$$

b) Connecting equations

supply connection:

$$T_i^{hot,in} = T_i^s \qquad i \in HXHS \qquad (4f)$$

$$T_i^{cold,in} = T_i^s \qquad i \in HXCS \qquad (4g)$$

internal connection:

$$T_i^{hot,out} - T_j^{hot,in} = 0 \qquad i \in HXHO, j \in HXHI \; (4h)$$

$$T_i^{cold,out} - T_j^{cold,in} = 0 \qquad i \in HXCO, j \in HXCI \; (4i)$$

target connection:

$$T_i^{hot,out} = T_i^t \qquad i \in HXHT \cup CUT \qquad (4j)$$

$$T_i^{cold,out} = T_i^t \qquad i \in HXCT \cup HUT \qquad (4k)$$

c) Lower and upper bounds of heat exchanged

lower bound:

$$-Q_i \leq 0 \qquad i \in PHX \cup CU \cup HU \qquad (4l)$$

upper bound: assuming constant thermal efficiency ($P_{h,i}$) and heat capacity flowrate (mC_P)

$$Q_i \leq P_{h,i}(mC_P)_i^{hot}(T_i^{hot,in} - T_i^{cold,in}) \qquad i \in PHX \cup CU \cup HU \qquad (4m)$$

where *PHX*: set of all process-process heat exchangers

CU: set of cold utility exchangers

HU: set of hot utility exchangers

HXHT: subset of *PHX* with hot side outlet is a controlled target

HXCT: subset of *PHX* with cold side outlet is a controlled target

CUT: subset of *CU* with outlet is a controlled target

HUT: subset of *HU* with outlet is a controlled target

HXHO: subset of *PHX* with hot side outlet entering a hot side inlet of the adjacent exchanger

HXCO: subset of *PHX* with cold side outlet entering a cold side inlet of the adjacent exchanger

HXHI: subset of *PHX* with hot side inlet coming from a hot side outlet of the adjacent exchanger

HXCI: subset of *PHX* with cold side inlet coming from a cold side outlet of the adjacent exchanger

HXHS: subset of *PHX* with hot side inlet directly coming from a hot supply

HXCS: subset of *PHX* with cold side inlet directly coming from a cold supply

$P_{h,i}$: thermal efficiency of exchanger *i*,

$$P_{h,i} = \frac{NTU_{h,i}(1 - e^{(NTU_{c,i} - NTU_{h,i})})}{NTU_{h,i} - NTU_{c,i}e^{(NTU_{c,i} - NTU_{h,i})}}$$

$$NTU_{h,i} = \frac{(UA)_i}{(mC_p)_i^{hot}}\ ,\ NTU_{c,i} = \frac{(UA)_i}{(mC_p)_i^{cold}}$$

$(mC_P)_i^{cold}$ and $(mC_P)_i^{hot}$: heat capacity flowrates on cold and hot sides of exchanger *i* (kW/^{o}C)

$(UA)_i$: product of heat transfer coefficient and area of exchanger *i* (kW/^{o}C)

The main "trick" used above to show that optimal operation of HENs is a LP problem is to introduce the thermal efficiency $P_{h,i}$ which avoids introducing the logarithmic mean temperature difference (LMTD) in the model for the heat transfer.

The efficiency factors are constant under the assumption of constant heat capacity flowrates (mC_P) and constant heat transfer coefficients (UA).

Example 1.1: A trivial HEN

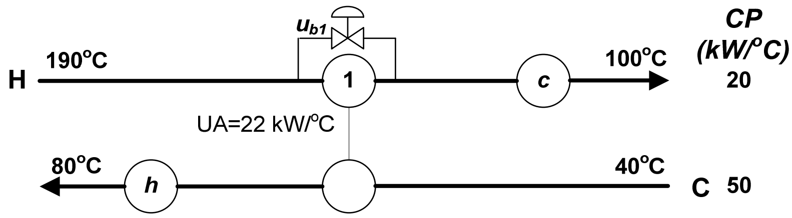


Figure 1 A trivial HEN

The HEN in Figure 1 contains one process exchanger and two utility types (N_U=2). Two outlet stream temperatures have targets (N_t =2). The dimensional space spanned by the manipulated variables in the inner HEN to the outer HEN (DS) is equal to 1 (see the calculation in Glemmestad, 1997). Using equation (2), we have $N_{DOF,U}=1+2-2=1$. This implies that there is one remaining degree of freedom for utility cost optimization. The meaning of $N_{DOF,U}$ can be described as follows:

The excess heat on the hot stream is equal to the sum of the duties of exchanger 1 (Q_1) and cooler (Q_c),

$$Q_1 + Q_c = 20(190\text{-}100) = 1800 \text{ kW}$$

while the required heat on the cold stream is equal to the sum of the duties of exchanger 1 and heater (Q_h),

$$Q_1 + Q_h = 50(80\text{-}40) = 2000 \text{ kW}$$

Hence, we have,

$$Q_h - Q_c = 2000\text{-}1800 = 200 \text{ kW}$$

This implies that Q_h is 200 kW more than Q_c. If only setpoint satisfaction (heat balances on the hot and cold streams) is required, then we can have several solutions (operating conditions) to satisfy Q_h-Q_c=200 and Q_1 to maintain the heat balances. However, to minimize utility cost, the solution with the lowest possible value of Q_c is preferred. From the information of the HEN, the maximum value of Q_1 (fully close of the bypass u_{b1}) is 1,827 kW which is enough to reject overall excess heat on the hot stream. Hence, Q_c can be assigned to zero while the bypass u_{b1} (Q_1) and Q_h are used for regulatory control to maintain the heat balances on the hot and cold streams. In this case, Q_c is the remaining degree of freedom at the constraint (zero utility duty) for optimality.

If the inlet temperature of hot stream increases to 200 ^{o}C, then the excess heat on the hot stream and the required heat on the cold stream can be written respectively by,

$$Q_1 + Q_c = 20(200\text{-}100) = 2000 \text{ kW}$$
$$Q_1 + Q_h = 50(80\text{-}40) = 2000 \text{ kW}$$

Hence, we have,

$$Q_h - Q_c = 0, \text{ or } Q_h = Q_c$$

This implies that Q_h is equal to Q_c. However, if the bypass of exchanger 1 is fully closed, we have $Q_{1,max}$=1,949 kW, which is less than the excess (required) heat on the hot (cold) stream. Hence, the lowest possible value of Q_c (or Q_h) is 51 kW to maintain the heat balance while u_{b1} is assigned to zero to maximize heat integration (or minimize utility cost). In this case, Q_h and Q_c are used for regulatory control, while u_{b1} is the remaining degree of freedom at the constraint (fully closed bypass) for optimality.

Using the same analysis, if the inlet temperature of hot stream increases to 210 ^{o}C, then to minimize utility cost, Q_c and u_{b1} should be used for regulatory control while Q_h is the remaining degree of freedom at the constraint (zero utility duty) for optimality. This example shows the cases that Q_c, $Q_1(u_{b1})$ and Q_h perform the remaining degree of freedom at constraints (active constraints) for optimality. □

An important property of a LP problem is that one optimal solution is always in a "corner". This implies that after satisfying in equality constraints (i.e. target temperatures), it is optimal to use all remaining degrees of freedom to satisfy active constraints (i.e. fully closing or opening of some bypasses or utility duties). Hence, Theorem 1 and Corollary 1.1 can be stated as follows:

Theorem 1 The optimal operation problem of simple HENs* is a LP problem

Proof: Equations 4a-4m

*simple HENs in this context refers to HENs with 1) only single bypasses (duties on individual process heat exchangers) and utility duties as degrees of freedom (manipulated variables), 2) given heat capacity flowrates, and 3) given *UA* values for the heat exchangers. Note that the process stream flowrates and stream-splits are not considered as degrees of freedom. □

Corollary 1.1 The optimal operation of simple HENs lies always at constraints

Proof: Property of a LP problem. □

The above LP problem may have multiple solutions (but not always) if there are some free degrees of freedom that may not affect the utility cost. This occurs when the HEN contains some loops. An idea for handling multiple solutions of the LP will be discussed in case study 1.2 of this thesis.

Note that it is possible to extend the LP formulation to include, for example, inequality constraints on temperatures (rather than targets) and other objective functions, for example, maximum temperature. However, the results in this research are based on the above formulation by use of split-range control.

The LP formulation implies that the optimal solutions are always at an intersection of constraints (vertex). The inequality constraints in the above LP formulation (equations 4l-4m) imply that active constraints occur on manipulated variables (i.e. zero or maximum duties of individual process and utility exchangers). Hence after the necessary degrees of freedom (manipulated variables) are used for control of the target temperatures (equality constraints), it is optimal to keep all remaining manipulated variables at constraints. However, under the variation of operating conditions, the optimal vertex (set of active constraints) may change. For a given operating window, we may have several optimal vertices for active constraint regions. Hence, to obtain optimality, one needs a good control policy for tracking the change of active constraints during the operation. One solution is to use an online optimization technique (Arkun and Stephanopoulos, 1980). Alternatively, one may try to avoid an online optimization task by using some logic to determine switching between active constraint regions and combine this with decentralized control. A particular implementation using common split-range control is the focus of this research.

2. Switching between active constraints

This section describes possible methods to implement the optimal policy by tracking the changing set of active constraints. The assumptions are:

Assumption A1: Target temperatures are feasible for the given disturbance window (output constraints do not change).

Assumption A2: The output constraints do not change and are always active. The optimal point is a vertex, i.e., at the intersection of constraints, and hence a certain number of inputs are at the constraints.

Under these assumptions, the optimal solution has the following properties:

a) The set of active constraints remains constant in a certain region of the disturbance space. The largest region in the disturbance space where the set of active constraints remains the same is known as critical region. Critical regions are polyhedral in shape for a LP and can be determined using off-line optimization or parametric programming tools (Kvasnica *et al.*, 2004).

b) If there are two or more critical regions in the given disturbance window, from the definition of critical region, it follows that the set of constraints are different. Since the output constraints do not change, it follows that the set of input constraints are different in each critical region. At the interface between two neighboring critical regions, constraints corresponding to both critical regions are active (which is a degenerate LP solution). However, since this constitutes a set of measure zero (i.e., the probability of being exactly on the boundary is zero), it does not affect the controllability properties of the network on the whole.

Using these properties of the optimal solution, it is possible to operate the HEN optimally using the following procedure:

a) In a given critical region R_o, it is possible to operate the HEN optimally using a decentralized control structure where some manipulated variables are used to control the output constraints using SISO control loops with zero steady state error, for example, PI controllers. The remaining manipulated variables are maintained at the constraints.

b) If the disturbances are such that we have moved from R_o to a different region R_1, it is possible to implement the optimal policy in R_1 by tracking the transition or change in active constraints.

Supposing that a system comprises of 3 manipulated variables and 2 controlled variables (target temperatures, T1 and T2). Clearly, 2 manipulated variables are needed for control. Furthermore, since one optimal solution is always at input constraints, the remaining manipulated variables may be at constraints (saturated). For a given operating window, active constraint regions can be found by parametric programming and the results are summarized as shown in Table 2 and Figure 2.

Table 2 Set of active constraints for example process

Region	**MV_1**	**MV_2**	**MV_3**
1	S	U	U
2	U	U	S
3	U	S	U

U-Unsaturated manipulated variable (inactive constraint) to be used for control of target temperatures

S-Saturated manipulated variable (active constraint)

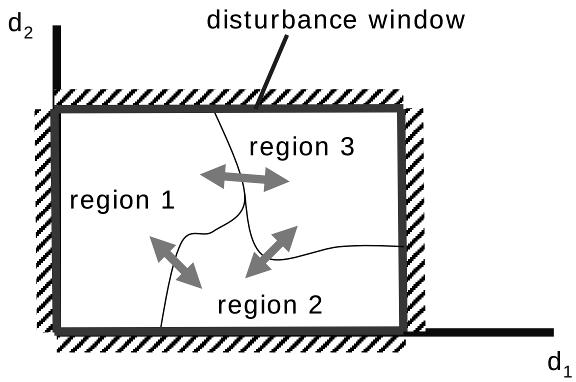


Figure 2 Active constraint regions

Thus, in region 1, it is optimal to use MV_2 and MV_3 to control the outputs T1 and T2 respectively using SISO PI control loops and keep MV_1 at constraint. When moving into region 2, MV_3 saturates and so, the optimal policy is to keep MV_3 at the constraint and instead use MV_1 as a manipulated variable for control. Thus MV_1 and MV_2 are used for control in region 2. Likewise, in region 3, the optimal policy is to control T1 and T2 using MV_1 and MV_3 and keep MV_2 at constraint. It is possible to keep tracking the regions under the changes in active constraints. When the new region is determined, the optimal policy corresponding to the new region is implemented. We discuss two ways to implement this policy:

a) Implementation 1: using switching logic

In this method, a switching logic based on the current state and change in some set of active constraints is used to determine the corresponding control law. The switching logic can be represented as:

(1) Switching between regions 1 and 2:
- MV_3 becomes active constraint in region 2
- MV_1 becomes active constraint in region 1

(2) Switching between regions 1 and 3:
- MV_2 becomes active constraint in region 3
- MV_1 becomes active constraint in region 1

(3) Switching between regions 2 and 3:
- MV_2 becomes active constraint in region 3
- MV_3 becomes active constraint in region 2

This switching logic with three sets of decentralized controllers (corresponding to regions 1, 2, and 3) can be used to implement the operating policy and is optimal in the presence of disturbances without the need to directly measure the disturbances and re-optimize the plant. The logic can be extended to more general situations using finite state machines.

However, in general, the switching logic can become very complicated. In some circumstances, a simpler implementation is possible using a split range controller. In the remainder of this thesis, the implementation of the optimal solution using this controller type will be focused.

b) Implementation 2: using split range control

Split range controllers are commonly used to control two or more manipulated variables with a single controller. A technique using structural information (sign matrix) to find a control structure for optimal operation of HENs was proposed by Mathisen (1994) and Glemmestad *et al.* (1996). They commented that in most cases the resulting control structure can be implemented in a split-range control manner. When two manipulated variables are used in a split-range controller, one of them is referred as primary manipulated variable and the other as a secondary manipulated variable. The primary manipulated variable can be thought of as the manipulated variable that is used to control a target under the nominal condition. However, the final choice of primary and secondary manipulated variables can be based on other considerations also. This flexibility will be exploited in the final control structure design.

A simple illustration will be provided for the above example. Assume that one split-range controller contains only two manipulated variables and region 1 is the "primary" region. Then MV_2 and MV_3 are the "primary" manipulated variables used for control of the target temperatures. For optimality, the active constraint should be switched to MV_3 when the operation moves into region 2, and to MV_2 in region 3. In terms of control, when moving into region 2, MV_1 needs to take over the task of saturated MV_3 ("MV_1 is used as a secondary manipulated variable for MV_3"), and when moving into region 3, MV_1 needs to take over the task of saturated MV_2 ("MV_1 is used as a secondary manipulated variable for MV_2"). Hence, we should combine MV_2 & MV_1 and MV_3 & MV_1 as split-range pairs and assign MV_1 as the secondary manipulated variable. This control system can be shown in Figure 3.

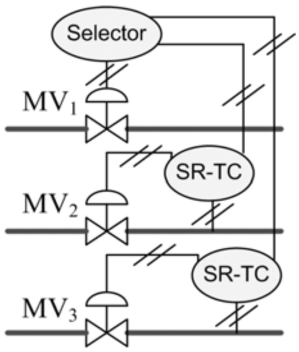


Figure 3 Control system of the example process (SR-TC = split-range temperature controller)

To illustrate more clearly how split-range control can be implemented for optimal operation, an application of split-range control to a furnace system as shown in Figure 4 will be described here. There are two types of fuel (fuel A and fuel B) for using in the furnace. Fuel A is cheaper than Fuel B. Hence, to operate the furnace in an optimal manner (minimizing fuel cost), fuel A should be used in the nominal condition while fuel B should be used only when necessary (e.g. the flow of fuel A reaches the upper limit). When fuel A is in use, the flow of fuel B presents the active constraint (saturated) at the lower bound. Likewise, when fuel B is in use (i.e. the flow of fuel A reaches the upper bound), the flow of fuel A presents the active constraint (saturated) at the upper bound. This optimal operation can be implemented using split-range control.

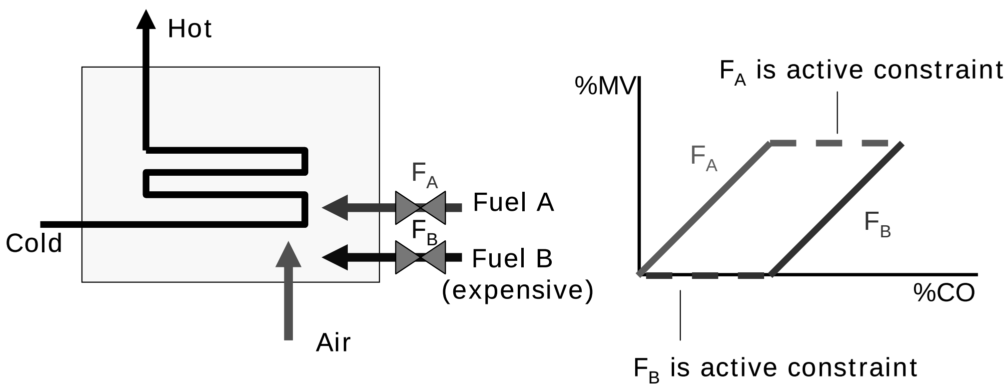


Figure 4 Application of split-range control to a furnace system

3. Determination of optimal split-range control structure

Referring to the examples in the previous section, the choices of secondary manipulated variables for primary manipulated variables could be determined by inspection. In general problems, with a large number of manipulated variables and active constraint regions, this is not a trivial task. Hence, a systematic method of determining this pairing is needed. This research proposes two approaches for determining optimal split-range control structure. In the first approach, one first identifies the set of nominal active constraints and then uses the information of directional effects (arithmetic signs) among manipulated variables and controlled variables to determine optimal split-range control structure. However, the control structure cannot guarantee optimality in some cases such as when a sign is unclear. Hence, the second approach based on an optimization formulation to determine an optimal split-range control structure is further developed. However, the information of all active constraint regions in a given disturbance space is additionally required.

3.1 Approach 1: Directional effects to determine optimal split-range control structure

If we define the directional effects of manipulated variables to controlled variables by arithmetic signs:

[+] = increasing MV increases CV
or decreasing MV decreases CV
[−] = increasing MV decreases CV
or decreasing MV increases CV
[±] = increasing (or decreasing) MV may increase or decrease CV
[0] = increasing (or decreasing) MV has no effect to CV

and the multiplication of sign elements:

[+].[+] = [+]

[−].[−] = [+]

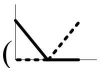
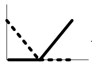
[+].[−] = [−]

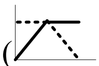
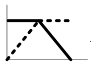
[+].[0] = [−].[0] = [±].[0] = [0]

[±].[+] = [±].[−] = [±].[±] = [±]

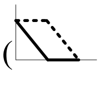
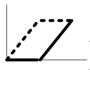
then the relationship between the directional effects of manipulated variables to controlled variables and split-range signal can be summarized as follows:

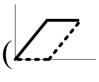
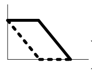
a) MV_1 and MV_2 have opposite directional effect to CV (Multiplication result of directional effect of MV_1 and MV_2 to CV is [−]).

Type I: Lower constraint switching ( or ), this split-range combination happens when two manipulated variables switch to their lower constraints.

Type II: Upper constraint switching ( or ), this split-range combination happens when two manipulated variables switch to their upper constraints.

b) MV_1 and MV_2 have same directional effect to CV (Multiplication result of directional effect of MV_1 and MV_2 to CV is [+]).

Type III: Lower and upper constraint switching ( or ), this split-range combination happens when two manipulated variables switch to their constraints by MV_1 at lower constraint and MV_2 at upper constraint.

Type IV: Upper and lower constraint switching ( or ), this split-range combination happens when two manipulated variables switch to their constraints by MV_1 at upper constraint and MV_2 at lower constraint.

c) MV_2 cannot affect to the paired CV of MV_1 (Multiplication result of directional effect of MV_1 and MV_2 to CV is [0]). No split-range combination is needed.

d) The directional effect of MV_2 to the paired CV of MV_1 is unclear (Multiplication result of directional effect of MV_1 and MV_2 to CV is [±]). Split-range signal is unclear.

Note that MV_1 (▬)=the input is used under the nominal condition (i.e. inactive constraint under the nominal condition), MV_2 (- - -)=the input is unused under the nominal condition (i.e. active constraint under the nominal condition), and CV=controlled variable.

The procedure to determine an optimal split-range control structure using directional effects is as follows:

1. Calculate $N_{DOF,U}$ by using equation (2), and then go further to step 2 if $N_{DOF,U} > 0$.
2. Solve the LP utility cost optimization problem for the nominal condition.

   2.1 Nominally unsaturated manipulated variables (inactive constraints) are used as primary manipulated variables for control.

   2.2 Nominally saturated manipulated variables (active constraints) are used as secondary manipulated variables.
3. Find the directional effects of primary manipulated variables to the paired controlled-variables and the directional effects of secondary manipulated variables to controlled variables, and then generate split-range signals and see which secondary manipulated variables can be used to protect which primary manipulated variables from saturation at the lower or upper bounds.

   3.1 If a secondary manipulated variable can protect only one primary manipulated variable, a split-range controller is used.

3.2 If a secondary manipulated variable can protect more than one primary manipulated variable, a selective controller is additionally required.

4. Use the information in steps 2 and 3 for the control structure design.

The proposed procedure cannot guarantee the optimality in two cases: 1) some directional effects are unclear; and 2) more than one secondary manipulated variable can protect a primary manipulated variable from saturation at a constraint. The first case may happen when there are some loops in the HEN which can cause parallel opposing effects from manipulated variables to controlled variables. The second case may happen when there are several secondary manipulated variables and active constraints change very often. In the case that the optimality cannot be guaranteed, further additional information from an offline optimization with expected disturbance variations (i.e. set of active constraints) would be useful for the control structure design. This will be described in approach 2.

3.2 Approach 2: ILP formulation to determine split-range control structure

In addition to the assumptions A1-A2, in order to use approach 2, further assumptions made are:

Assumption A3: One split-range combination contains only two manipulated variables. Hence, each primary manipulated variable can have only one secondary manipulated variable. Note that this does not rule out the possibility that a variable treated as a secondary manipulated variable can be used in two or more split range controllers.

Assumption A4: Only one saturation (upper or lower bounds) is allowed for each manipulated variable

If the assumptions A1-A4 hold and the set of active constraints in the critical regions is known, then an integer linear programming (ILP) formulation for the design of an optimal split-range control structure can be formulated as follows:

Definition 1: Set of controlled and manipulated variables

CV: set of controlled variables, $CV = \{ \mathrm{CV}_1, \mathrm{CV}_2, \ldots, \mathrm{CV}_{\mathrm{N_{CV}}-1}, \mathrm{CV}_{\mathrm{N_{CV}}} \}$

MV: set of manipulated variables, $MV = \{ \mathrm{MV}_1,\ \mathrm{MV}_2, \ldots\ \mathrm{MV}_{\mathrm{N_m}-1},\ \mathrm{MV}_{\mathrm{N_m}} \}$

MVAAT: subset of *MV* with manipulated variables which are always active constraints (saturated at upper or lower bounds)

MVINAT: subset of *MV* with manipulated variables which are always inactive constraints (never saturated)

MVAT: subset of *MV* with manipulated variables which change between being active and inactive constraints

Definition 2: Primary and secondary manipulated variables

Primary manipulated variable is a manipulated variable that is used for controlling an output (target), except when it is saturated. Secondary manipulated variable is a manipulated variable that is used to take over the task of a saturated primary manipulated variable.

Definition 3: Relationship between primary and secondary manipulated variables

Let $x_{i,j}$ (where $i, j \in MV$) be a binary variable which represents the relationship between manipulated variable $\mathrm{MV_i}$ and manipulated variable $\mathrm{MV_j}$

for i=j, $x_{i,i}$ = 1 implies $\mathrm{MV_i}$ is a primary manipulated variable and $x_{i,i}$ = 0 implies $\mathrm{MV_i}$ is a secondary manipulated variable or unused

for $i \neq j$, $x_{i,j}$ = 1 implies $\mathrm{MV_j}$ is a secondary manipulated variable for $\mathrm{MV_i}$ and $x_{i,j}$ = 0 implies $\mathrm{MV_j}$ is not a secondary manipulated variable for $\mathrm{MV_i}$

Definition 4: Relative order between manipulated variables and controlled variables

Let $r_{k,j}$ be relative order between controlled variable $\mathrm{CV_k}$ and manipulated variable $\mathrm{MV_j}$. Relative order is a structural measure of how direct an effect an input has on an output (Daoutidis and Kravaris, 1992). However, we here assume $r_{k,j}$ as the number of exchangers between controlled variable $\mathrm{CV_k}$ and manipulated variable $\mathrm{MV_j}$

Definition 5: Relationship between controlled variables and manipulated variables

Let $z_{k,j}$ (where $k \in CV, j \in MV$) be a binary variable that represents the relationship between controlled variable $\mathrm{CV_k}$ and manipulated variable $\mathrm{MV_j}$

$z_{k,j}$ = 1 implies controlled variable $\mathrm{CV_k}$ is paired with manipulated variable $\mathrm{MV_j}$ and $z_{k,j}$ = 0 implies controlled variable $\mathrm{CV_k}$ is not paired with manipulated variable $\mathrm{MV_j}$

Objective function I: Minimizing the number of “inter-connection” or “complexity” of control structure (or minimizing unnecessary relationships between primary and secondary manipulated variables)

$$\min J_I = \sum_{i \in MV} \sum_{j \in MV, j \neq i} x_{i,j} \tag{5}$$

Constraint 1: Assign one primary manipulated variable to each control objective

The number of primary manipulated variables is equal to the number of controlled variables (N_{CV})

$$\sum_{i \in MV} x_{i,i} = N_{CV} \tag{6}$$

Constraint 2: A manipulated variable MV_i that is always an active constraint should not be used for other purposes

Manipulated variable MV_i is not used for control

$$x_{i,i} = 0 \qquad i \in MVAAT \tag{7}$$

Manipulated variable MV_i has no need for a secondary manipulated variable

$$\sum_{j \in MV, j \neq i} x_{i,j} = 0 \qquad i \in MVAAT \tag{8}$$

Manipulated variable MV_i is not used as a secondary manipulated variable

$$\sum_{j \in MV, j \neq i} x_{j,i} = 0 \qquad i \in MVAAT \tag{9}$$

Constraint 3: A manipulated variable MV_i that is never an active constraint is used as a primary manipulated variable with no need for a secondary manipulated variable

Manipulated variable MV_i is a primary manipulated variable

$$x_{i,i} = 1 \qquad i \in MVINAT \qquad (10)$$

Manipulated variable MV_i has no need for a secondary manipulated variable

$$\sum_{j \in MV, j \neq i} x_{i,j} = 0 \qquad i \in MVINAT \qquad (11)$$

Manipulated variable MV_i is not used as a secondary manipulated variable

$$\sum_{j \in MV, j \neq i} x_{j,i} = 0 \qquad i \in MVINAT \qquad (12)$$

Constraint 4: A manipulated variable MV_i that changes between being an active and inactive constraint may be a primary or secondary manipulated variable.

if MV_i is chosen as a primary manipulated variable that can be saturated (active constraint), then a secondary manipulated variable is needed

$$\text{if } x_{i,i} = 1 \text{ then } \sum_{j \in MVAT, j \neq i} x_{i,j} = 1 \quad i \in MVAT$$

if MV_i is not chosen as a primary manipulated variable, then it has no need for a secondary manipulated variable

$$\text{if } x_{i,i} = 0 \text{ then } \sum_{j \in MVAT, j \neq i} x_{i,j} = 0 \quad i \in MVAT$$

the above two statements can be written

$$-x_{i,i} + \sum_{j \in MVAT, j \neq i} x_{i,j} = 0 \qquad i \in MVAT \qquad (13)$$

if MV_j is chosen as a primary manipulated variable, then it is not used as a secondary manipulated variable for other manipulated variables

$$\text{if } x_{j,j} = 1 \text{ then } \sum_{i \in MVAT, i \neq j} x_{i,j} = 0 \quad j \in MVAT$$

if MV_j is chosen as a secondary manipulated variable, then it is used for at least one primary manipulated variable

$$\text{if } x_{j,j} = 0 \text{ then } \sum_{i \in MVAT, i \neq j} x_{i,j} \geq 1 \quad j \in MVAT$$

the above two statements can be written

$$x_{j,j} + \sum_{i \in MVAT, i \neq j} x_{i,j} \geq 1 \qquad j \in MVAT \qquad (14)$$

$$M(x_{j,j} - 1) + \sum_{i \in MVAT, i \neq j} x_{i,j} \leq 0 \qquad j \in MVAT \qquad (15)$$

where M = a positive integer which is greater than the number of members in *MVAT*

Constraint 5: Possible and impossible split-range combination of manipulated variables (these constraints are obtained from the information of active constraint regions)

Constraint 5A: Impossible split-range combination of manipulated variables

"Impossible pair: two manipulated variables which are active constraints (saturated) at the same time cannot be combined as a split-range pair"

For an active constraint region *R*, we have

$$\sum_{i \in MVAT^{A,R}} \sum_{j \in MVAT^{A,R}, j \neq i} x_{i,j} = 0 \qquad R \in RS \qquad (16)$$

where $MVAT^{A,R}$ is the subset of *MVAT* with manipulated variables being active constraints in region *R*. *RS* is the set of active constraint regions.

Constraint 5B: Possible split-range combination of manipulated variables

"Possible pair: two manipulated variables which are not active (inactive) constraint at the same time may be combined as a split-range pair"

For an active constraint region *R*, we have

$$x_{j,j} + \sum_{i \in MVAT^{I,R}} x_{i,j} \geq 1 \qquad j \in MVAT^{A,R}, R \in RS \qquad (17)$$

$$x_{i,i} + \sum_{j \in MVAT^{A,R}} x_{j,i} \geq 1 \qquad i \in MVAT^{I,R}, R \in RS \qquad (18)$$

where $MVAT^{I,R}$ is the subset of *MVAT* with manipulated variables being inactive constraints in region *R*.

Combining objective function I and constraints 1-5, Problem P1 can be written,

Problem P1

$$\min J_I = \sum_{i \in MV} \sum_{j \in MV, j \neq i} x_{i,j}$$

subject to

equations 6 to 18

By solving Problem P1, one obtains split-range pairs that can provide optimal switching between active constraint regions. However, the solution of Problem P1 may be non-unique. Hence, relative orders are introduced as an additional criterion for screening the set of poorly controllable structure solutions. The additional objective function and constraints are as follows:

Objective function II: Minimizing the sum of relative orders of the control pairs

$$\min J_{II} = \sum_{k \in CV} \sum_{j \in MV} r_{k,j} z_{k,j} \qquad (19)$$

Constraint 6: Assign one manipulated variable to each control objective

$$\sum_{j \in MV} z_{k,j} = 1 \qquad k \in CV \qquad (20)$$

Constraint 7: Only primary manipulated variables are paired with controlled variables.

If MV_j is a primary manipulated variable, it must be paired with a controlled variable

$$\text{If } x_{j,j} = 1 \text{ then } \sum_{k \in CV} z_{k,j} = 1 \qquad j \in MV$$

If MV_j is not a primary manipulated variable, it must not be paired

$$\text{If } x_{j,j} = 0 \text{ then } \sum_{k \in CV} z_{k,j} = 0 \qquad j \in MV$$

therefore,

$$-x_{j,j} + \sum_{k \in CV} z_{k,j} = 0 \qquad j \in MV \qquad (21)$$

The ILP problem now concerns two objective functions that can be solved using lexicographic optimization. In lexicographic optimization, the objectives are arranged in decreasing order of preference; and objectives with a higher preference are considered to be infinitely more important than those with lower orders. Among the solutions that are optimal with respect to the first objective, solutions that are optimal with respect to the second objective are chosen.

Using the idea of lexicographic optimization, we first solve Problem P1:

$$J_I^* = \min_x J_I(x), \qquad x \in S$$

where S is the feasible set and then solve an associated Problem P1′:

$$\min_x J_{II}(x), \qquad x \in S,\ J_I = J_I^*(x)$$

which ensures that among the minimized J_I solutions, the minimized J_{II} solutions are chosen. In principle, we need to solve 2 optimization problems in sequence. However, it is possible to solve P1 and P1′ as a single optimization problem by minimizing a weighted objective function $wJ_I + J_{II}$, where w is a sufficiently large positive number chosen appropriately. Suggestions for choice of w are given in Sherali (1982), and Sherali and Soyster (1983). Hence, we solve the following Problem P2:

Problem P2

$$J = \min(wJ_I + J_{II})$$
$$J_I = \sum_{i \in MV} \sum_{j \in MV, j \neq i} x_{i,j} \ , \ J_{II} = \sum_{k \in CV} \sum_{j \in MV} r_{k,j} z_{k,j}$$

subject to

equations 6 to 21

It can be seen that constraints 6 and 7 (equations 20 and 21) do not alter the feasible set for the ILP Problem P1. The ILP Problem P2 consists of two objective functions with a weighting factor (*w*) between the two. The first objective is used to minimize complexity when changing between active constraints whereas the second objective (controllability) is used to select the most controllable control structure. A large value of *w* will imply that the second objective (controllability) will only be considered when there are multiple solutions.

It is possible for the ILP to have no feasible solution, that is, no optimal split-range control structure can be found. This may happen when there are conflicts among the equations in constraint 5. In this case, an online optimization may be suggested for implementing optimal operation.

Part II: HENs synthesis with controllability improvement

4. Structural controllability evaluation

To assess controllability of HENs, the dynamic models of heat exchangers and heat exchanger networks are needed. In this section, a simplified dynamic model of heat exchangers for using in structural analysis is proposed and then extended for the structural analysis of heat exchanger networks.

4.1 Structural model of heat exchangers

Although in fact heat exchangers should be described by a distributed model such as multi-cell model (Mathisen, 1994), for structural analysis a lumped (mixing tank) model is assumed in this work.

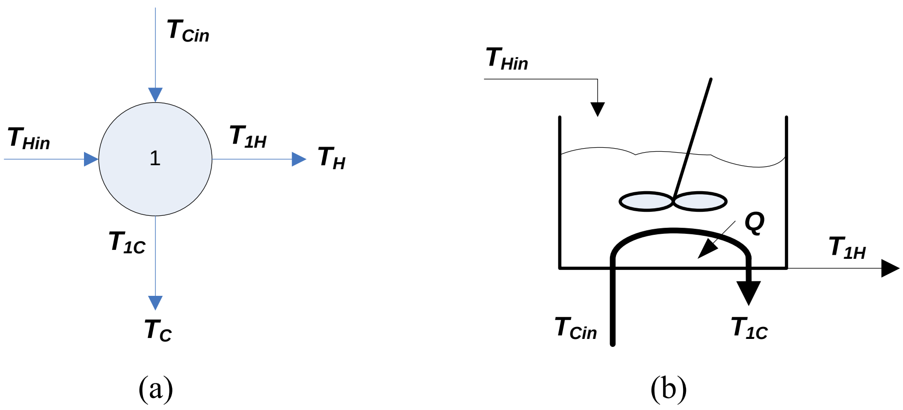


Figure 5 (a) heat exchanger and (b) mixing tank model

If a heat exchanger in Figure 5a is supposedly described by a mixing tank model with a cooling coil in Figure 5b, the energy balance around the hot side can be written:

$$\rho_H V_H C_{PH} \frac{dT_{1H}}{dt} = \rho_H F_H C_{PH} \left[T_{Hin} - T_{1H}\right] - Q \qquad (22)$$

Likewise, if a mixing tank with a heating coil is considered, the energy balance around the cold side can be written:

$$\rho_C V_C C_{PC} \frac{dT_{1C}}{dt} = \rho_C F_C C_{PC} \left[T_{Cin} - T_{1C}\right] + Q \tag{23}$$

where *state variables* are outlet temperatures on the hot and cold sides (T_{1H} and T_{1C}), *input variables* are inlet temperatures on the hot and cold sides (T_{Hin} and T_{Cin}) and duty of heat exchanger (Q), *process parameters* are density of fluid (ρ_H, ρ_C), volumes of the compartments of the exchanger (V_H, V_C), heat capacity of fluid (C_{PH}, C_{PC}) and volumetric flowrates (F_H, F_C) on the hot and cold sides, *output variables* are the outlet temperatures of the hot and cold streams (T_H and T_C) which can be written:

$$T_H = T_{1H} \tag{24}$$

$$T_C = T_{1C} \tag{25}$$

Although a (single) bypass should be considered as a manipulated variable, to simplify the model, the duty of a heat exchanger is assumed as a manipulated variable. Hence, based on the model in equations 22 and 23, only one outlet temperature of a heat exchanger can have a target. The structural system matrix $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$ of a process heat exchanger with the target T_H can be shown in Table 3.

Table 3 Structural system matrix of a process heat exchanger

	T_{1H}	T_{1C}	Q
T_{1H}	x		x
T_{1C}		x	x
T_H	x		

The element 'x' in the matrix denotes that the column variable shows some physical relationship with the row variable. For example, the input Q can affect the output T_H through the path Q -->T_{1H} -->T_H.

For hot (or cold) utility exchangers, there is only one state variable (i.e. the outlet temperature of the exchanger on the process stream side) to be considered, hence, the structural system matrix can be obtained from the energy balance around the exchanger on the process stream side.

4.2 Structural model of heat exchanger networks

Mathisen (1994) showed that the important model features of heat exchanger networks are 1) structure, 2) residence time, and 3) model order of bypasses and connecting pipes. However, in structural analysis, only the structure of HENs will be considered. The structure of HENs is very important because it determines the relationships among input/output variables of heat exchangers in the network. Some input variables (i.e. inlet temperatures of heat exchangers) in a heat exchanger model are considered as state variables in a heat exchanger network model. Furthermore, only some outlet temperatures of heat exchangers can have targets (i.e. typically the temperatures concerning the outlet of process streams). In this work, the structural model of HENs is given by combining structural models of heat exchangers in the network. The additional assumption is that the dynamics of stream splitters and stream mixers are fast and, hence, are neglected.

4.3 Structural analysis tools

The term 'structural controllability' in this context implies the inherent control property of a HEN with a decentralized control system independent of the controller type. The control system will be determined based on the criteria of structural singularities, parallel opposing effects, relative orders, and decoupling indices as demonstrated in the following sections.

4.3.1 Structural singularity

Inputs in heat exchanger networks only affect the outputs if there is a "downstream path" (Linnhoff and Kotjabasakis, 1986) between the input and the output. The lack of a downstream path yields structural singularity. The control system with structural singularity must be avoided because the system becomes uncontrollable. Structural singularity of HENs can be addressed by checking the number of degrees of freedom or the rank of the transfer matrix of the system (Glemmestad, 1997). However, this is based on the assumption that all manipulated variables are used for control. Since this work assumes single-input/single-output (SISO) pairings are used for control, structural singularity will be addressed by the rank of the transfer matrix of the selected manipulated variables.

Note that for structurally controllable HENs, there will be at least one SISO control system without structural singularity.

Example 4.1: A SISO control system without structural singularity

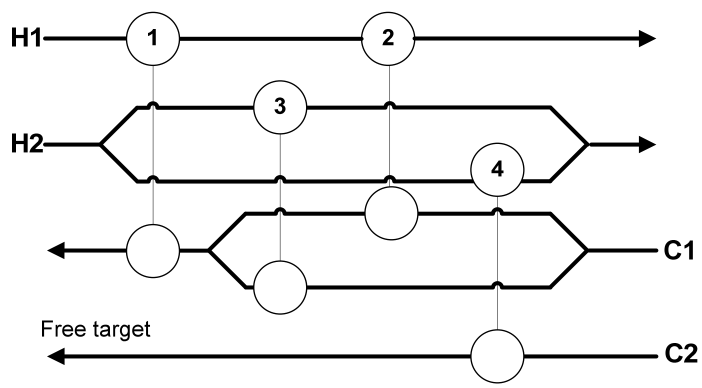


Figure 6 Heat exchanger network in example 4.1

The target temperatures of the HEN in Figure 6 are the outlet temperatures of streams H1, H2, and C1 (T_{H1}, T_{H2}, T_{C1}) while the outlet temperature of stream C2 is free. The candidates of manipulated variables for control are the duties of individual heat exchangers (Q_1, Q_2, Q_3 and Q_4).

In general, before designing a control system, one should first see whether the HEN itself has structural singularity or not. This can be checked using energy balance around the HEN (Glemmestad, 1997),

$$\begin{aligned}(F_{H1}C_{p,H1})(T_{H1}^{sp}-T_{H1}^{in}) &= -Q_1 - Q_2\\(F_{H2}C_{p,H2})(T_{H2}^{sp}-T_{H2}^{in}) &= -Q_3 - Q_4\\(F_{C1}C_{p,C1})(T_{C1}^{sp}-T_{C1}^{in}) &= Q_1 + Q_2 + Q_3\end{aligned} = \underbrace{\begin{bmatrix}-1 & -1 & 0 & 0\\0 & 0 & -1 & -1\\1 & 1 & 1 & 0\end{bmatrix}}_{G_{sys}}\begin{bmatrix}Q_1\\Q_2\\Q_3\\Q_4\end{bmatrix} \quad (26)$$

Because rank(G_{sys}) = 3, the HEN is structurally controllable. This also implies that there will be at least one SISO control system without structural singularity.

Three manipulated variables are required for SISO control and this results in four possible sets of manipulated variables: $\{Q_1, Q_2, Q_3\}$, $\{Q_1, Q_2, Q_4\}$, $\{Q_1, Q_3, Q_4\}$ and $\{Q_2, Q_3, Q_4\}$. However, only the sets without structural singularity are preferred. Structural singularity of a SISO control system can be checked by considering the rank of the corresponding transfer matrix.

For the set $\{Q_1, Q_2, Q_3\}$, the column corresponding to Q_4 is removed,

$$G_{c,4} = \begin{bmatrix}-1 & -1 & 0\\0 & 0 & -1\\1 & 1 & 1\end{bmatrix} \quad (27)$$

where $G_{c,i}$ is the transfer matrix G_{sys} with the removal of the *i*th column

Because of rank($G_{c,4}$) = 2, the set $\{Q_1, Q_2, Q_3\}$ has rank deficiency and exhibits structural singularity. The ranks for all possible sets of manipulated variables are summarized in Table 4. The result shows that the sets $\{Q_1, Q_3, Q_4\}$ and $\{Q_2, Q_3, Q_4\}$ do not exhibit structural singularity.

Table 4 Ranks of potential sets of manipulated variables

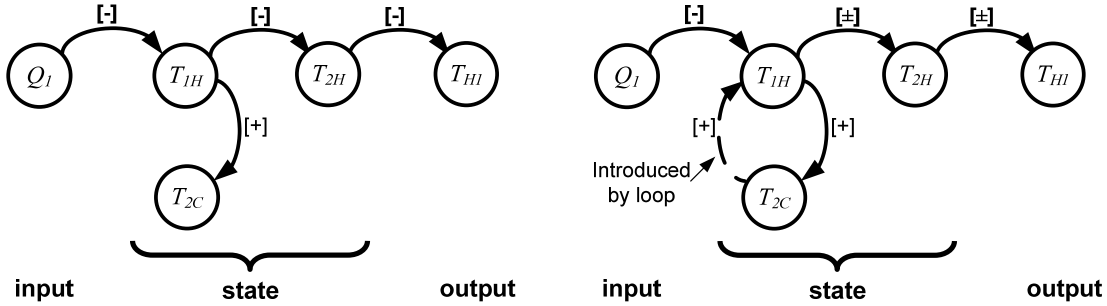
Manipulated Variables	$\{Q_1, Q_2, Q_3\}$	$\{Q_1, Q_2, Q_4\}$	$\{Q_1, Q_3, Q_4\}$	$\{Q_2, Q_3, Q_4\}$
Rank	2	2	3	3

4.3.2 Right half plane zero (RHP-zero)

RHP-zeros represent a fundamental limitation of the achievable control performance and should be avoided in the control system design (Rosenbrock, 1970). RHP-zeros may occur if inputs have parallel opposing effects to outputs. For HENs, this may occur when there are heat load loops in the network (Mathisen, 1994).

Example 4.2: Parallel opposing effects and RHP-zeros

Refer to the HEN in Figure 6, heat exchangers 1 and 2 are parts of a heat load loop. Hence, some manipulated variables may have parallel opposing effects to target temperatures. A digraph with directional effects (denoted by arithmetic signs) of the path from Q_1 to T_{H1} is used to indicate the problem of a heat load loop as shown in Figure 7.



(a) with no heat load loop (b) with a heat load loop

Figure 7 Digraph of the path from Q_1 to T_{H1}

$\xrightarrow{[+]}$ denotes increasing (decreasing) the value of the variable at the input node (Q_1) increases (decreases) the value of the variable at the pointed node

$\xrightarrow{[-]}$ denotes increasing (decreasing) the value of the variable at the input node (Q_1) decreases (increases) the value of the variable at the pointed node

$\xrightarrow{[\pm]}$ denotes increasing or decreasing the value of the variable at the input node (Q_1) may increase or decrease the value of the variable at the pointed node

As shown in Figure 7a, there is only one effect from Q_1 to T_{1H} when the HEN has no loop. However, if there is such a loop presented, an additional opposing effect (see Figure 7b) may introduce parametric singularity and RHP-zeros to the controlled output T_{H1}. □

4.3.3 Relative order and decoupling index

Daoutidis and Kravaris (1992) reviewed a useful structural property of a general system: concept of relative order and its relationship with the digraph technique. Relative order (structural time delay) can be used as a structural measure to evaluate how direct an effect an input has on an output (physical closeness). The idea is that if the input is physically close to the output, then favorable static and dynamic characteristics for the particular input/output pair is possible. In addition, a relative order matrix can also provide an insight on the inherent structural coupling in the process.

One simple way to find the value of relative order $r_{k,j}$ between input j and output k is to use the information from a digraph technique. The length of the shortest path ($l_{k,j}$) between input j and output k can be used to find the value of relative order $r_{k,j}$ as follows:

$$r_{k,j} = l_{k,j} - 1 \qquad (28)$$

A square relative order matrix for a decentralized control system can be defined as:

$$[r_{k,j}] = \begin{bmatrix} r_1 & r_{1,2} & \cdots & r_{1,m} \\ r_{2,1} & r_2 & \cdots & r_{2,m} \\ \vdots & \vdots & \ddots & \\ r_{m,1} & r_{m,2} & \cdots & r_m \end{bmatrix} \quad (29)$$

where the diagonal elements r_k is relative order of the control pair k.

To perform control pairing selection, Soroush (1996) proposed the direct effect determination by the concept of smallest sum of relative order ($RO = \sum_k r_k$). In addition, the difference of magnitude of r_k and $r_{k,j}$ can be used to determine the degree of interaction of the selected control system. Lee *et al.* (2001) defined the term "decoupling index" (*DI*) as a structural measure of degree of decoupling for a control system that can be calculated by

$$DI = \sum_k \sum_{j \neq k} \frac{r_k}{r_{k,j}} \quad (30)$$

Smaller value of *DI* implies that the control system is more structurally decoupled. This is corresponding with the work of Holt and Morari (1985) that the interaction can be reduced by the increase of time delays on off-diagonal elements in multivariable systems.

Example 4.3: Relative orders and decoupling index of a HEN

The HEN in Figure 6 is considered here again. Because there are two alternative sets of manipulated variables for control, further analysis is required to select the best one. Relative orders and decoupling index will be used for this purpose.

The digraph in Figure 7b shows that the shortest path from Q_1 to T_{H1} is $Q_1 \rightarrow T_{1H} \rightarrow T_{2H} \rightarrow T_{H1}$. According to equation (28), the relative order of this pair is 3-1=2. The square relative order matrix for each alternative set of manipulated variables is shown in Table 5. The result shows that the set {Q_2, Q_3, Q_4} is more favorable in sense of direct effect and interaction.

Table 5 Square relative order matrix for each possible set of manipulated variables

	Q_1	Q_4	Q_3	Q_2	Q_4	Q_3
T_{H1}	2	∞	3	1	∞	3
T_{H2}	∞	1	1	∞	1	1
T_{C1}	1	∞	2	2	∞	2
	RO=2+1+2=5, *DI*=2/3+1/1+2/1=3.67			*RO*=1+1+2=4, *DI*=1/3+1/1+2/2=2.33		

□.

Note that the value of relative order can also be obtained by counting the number of exchangers between a manipulated input and a target temperature. For example, there are two exchangers (one heat exchanger and one cooler) between Q_1 and T_{H1}, hence, the relative order is 2.

Note further that the best value of *RO* is equal to the number of target temperatures, that is, a direct effect is possible for all control pairs. The best value of *DI* is zero, that is, the control system is totally decoupled. In general, poor *RO* usually reflect to poor *DI*.

4.4 Structural controllability evaluation for HENs

The structural controllability analysis of HENs in this research is defined as the evaluation of the best potential control pairing based on the criteria of structural singularity, parallel opposing effects, relative orders, and decoupling index. In this section, the idea of structural controllability evaluation of HENs is discussed and formulated as an integer linear program (ILP).

4.4.1 General concept of structural analysis (for control system design)

In structural analysis, one should first look for control systems without structural singularity because this is a necessary condition for a controllable system (Rosenbrock, 1970). However, this usually results in several alternatives of control systems. Hence, some controllability criteria should be applied for screening the potential control system. This research proposed to use relative orders, number of parallel opposing effects, and decoupling index as the criteria for the screening. In general, this can be done through a step-by-step consideration of each controllability criterion in a preference order, and then the best potential control system is found. Figure 8 shows the consideration steps of structural analysis for the control system design. Note that if the consideration order of controllability criteria is changed, then different solutions may be obtained.

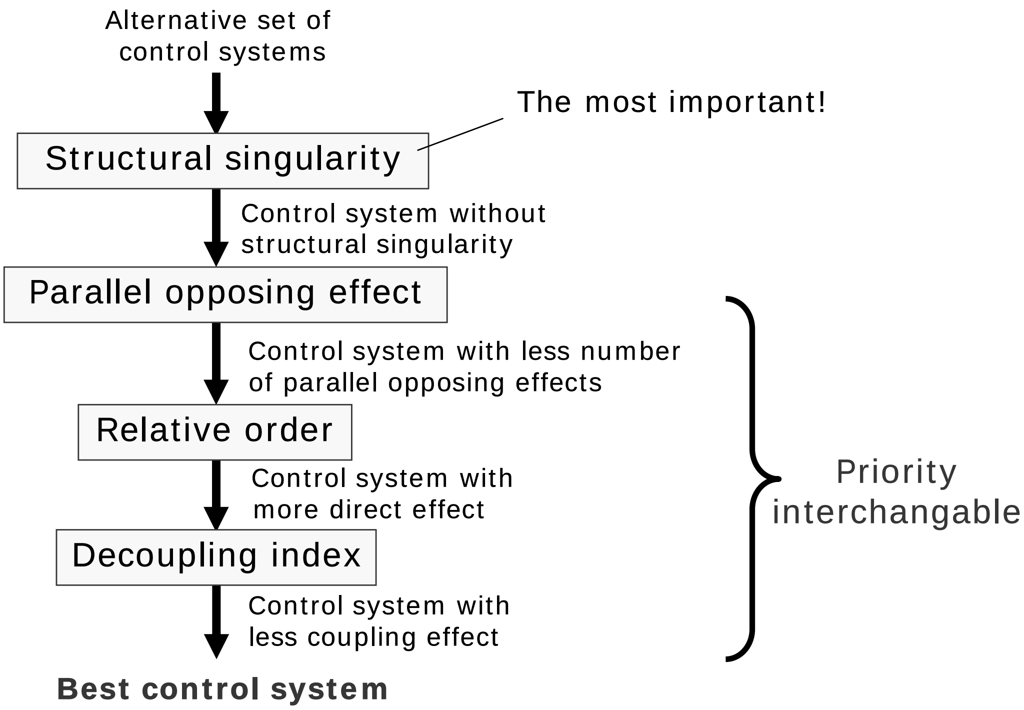


Figure 8 Steps of structural analysis for control system design

4.4.2 ILP for structural controllability evaluation

As described, time delays and RHP-zeros should be avoided and minimized in the control system. This can be structurally proposed as the minimization of the two objectives: the sum of relative orders (*RO*) and the number of parallel opposing effects (N_{POE}). In addition, system interactions also limit the control performance. Hence, decoupling index (*DI*) should also be taken into account as the third objective in the optimization. As poor *RO* usually reflects to poor *DI*, *RO* will be considered as the most important objective in the optimization. Furthermore, interactions often introduce only a minor control problem in HENs (Mathisen, 1994); hence, *DI* is considered as the least important objective.

Because of the possibility of the conflict among the objectives (i.e. improving one may worsen the other) and the difficulty to assess and compare the objectives, the problem is here assumed as a preemptive ordering type (Kornbluth, 1973), that is, there exists a preference order of the objective functions. Two techniques named lexicographic ordering and one-dimensional methods (Yu, 1975) can be applied to this problem. The first technique starts with minimizing the primary objective in which its optimal value is considered as an equality constraint during the minimization of the second objective, and so on. This technique requires a sequence of single objective optimization. In the latter technique, one introduces a utility function such as a linear-weighting function $u[f_1(x),..., f_n(x)] = \sum_i^n w_i f_i(x)$, where w_i is a non-negative weight, and then minimizes it as a single optimization problem. However, this approach requires the appropriate values of w_i to have $w_1 f_1(x) >> w_2 f_2(x) >> ...... >> w_n f_n(x)$. A method for determining these values can be found in Sherali and Soyster (1983). This work chose to use a linear-weighting function to handle the multi-objective optimization problem as shown in the following:

Assumptions:

1. The considered HEN is structurally controllable
2. One manipulated variable is paired with only one controlled variable
3. A manipulated variable is considered in terms of 'duty of an individual heat exchanger'

Sets:

MV denotes set of manipulated variables

MVS^n denotes set of manipulated variables in the SISO control system n that exhibits structural singularity, $n = 1, 2, ..., N_{cs,sin}$

$N_{cs,sin}$ = the number of SISO control systems with structural singularity

CV denotes set of controlled variables

Indices:

$i, j \in MV$

$m \in MVS^n$

$k \in CV$

Binary variables:

$z_{k,j}$ = 1 denotes that input j is paired with output k

= 0 denotes that input j is not paired with output k

$d_{k,i,j}$ = 1 denotes that the term $\frac{r_{k,i}}{r_{k,j}}$ is used in the calculation of DI

= 0 denotes that the term $\frac{r_{k,i}}{r_{k,j}}$ is not used in the calculation of DI

Parameters:

$r_{k,j}$ denotes relative order between input j and output k

$p_{k,j}$ = 1 if input j has parallel opposing effects to output k

= 0 if input j has no parallel opposing effect to output k

Three objective functions are formulated with a linear-weighting function to minimize the sum of relative orders (*RO*), the number of parallel opposing effects (N_{POE}), and decoupling index (*DI*). Four constraints are considered:

Constraint 1: Assign one manipulated variable to each controlled variable
Constraint 2: One manipulated variable cannot be assigned to more than one controlled variable
Constraint 3: Only the terms $\frac{r_{k,i}}{r_{k,j}}$ related to the selected manipulated variables are used for the calculation of decoupling index
Constraint 4: Avoid the control systems with structural singularity (need to check the rank of all possible sets of manipulated variables)

These statements are translated into an optimization Problem P3, resulting in an integer linear programming problem for control structure synthesis of HENs based on structural information.

Problem P3

$$min\ w_1 \underbrace{\sum_{k\in CV}\sum_{j\in MV} z_{k,j} r_{k,j}}_{\text{the sum of relative order } (RO)} + w_2 \underbrace{\sum_{k\in CV}\sum_{j\in MV} z_{k,j} p_{k,j}}_{\text{the number of parallel opposing effects } (N_{POE})} + w_3 \underbrace{\sum_{k\in CV}\sum_{i\in MV}\sum_{j\in MV, j\neq i} d_{k,i,j} \frac{r_{k,i}}{r_{k,j}}}_{\text{decoupling index } (DI)} \quad (31a)$$

s.t.

$$\sum_{j\in MV} z_{k,j} = 1 \qquad j \in MV \qquad (31b)$$

$$\sum_{k\in CV} z_{k,j} \leq 1 \qquad j \in MV \qquad (31c)$$

$$d_{k,i,j} \geq z_{k,i} + \sum_{k\in CV} z_{k,j} - 1 \qquad k \in CV,\ i,j \in MV,\ j \neq i \qquad (31d)$$

$$\sum_{m\in MVS^n}\sum_{k\in CV} z_{k,m} \leq N_{CV} - 1 \qquad n = 1, 2, \ldots, N_{cs,sin} \qquad (31e)$$

The control systems with structural singularity are eliminated by constraint 4 (equation 31e) that can be obtained from the information of the ranks of all possible sets of manipulated variables. The solution from the optimization can propose a best potential control system corresponding to the preference order of the three objectives. Furthermore, the values of the three objectives: *RO*, N_{POE}, and *DI*, can be used as structural indicators for the selection of the most controllable HEN among the set of HEN alternatives. The implementation of the ILP Problem P3 is shown in Figure 9.

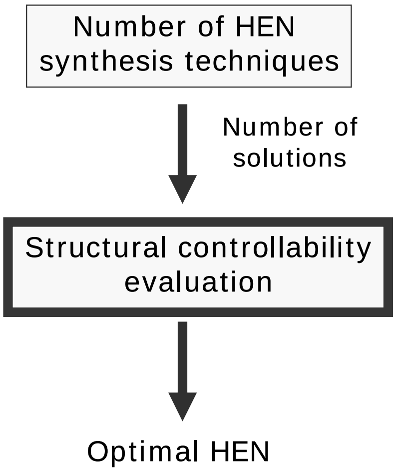


Figure 9 Implementation of structural controllability evaluation for screening the most controllable HEN

5. HEN synthesis with user-specified number of subnetworks

Among the HEN structure solution sets, there may be some promising solutions with a number of subnetworks. One possible way to enforce the solution to have subnetworks is to limit the number of matches to the minimum. In general, the minimum number of matches ($N_{unit,min}$) can be calculated by (Linnhoff *et al.*, 1979),

$$N_{unit,min} = N_s - N_{sub} \quad (32)$$

where N_s is the number of streams and N_{sub} is the number of subnetworks.

By introducing a constraint to limit the upper bound of the number of matches into the model of Yee and Grossman (1990),

$$\sum_{i \in HP} \sum_{j \in CP} \sum_{st \in ST} y_{i,j,st} \le N_{unit,\min} \tag{33}$$

where $y_{i,j,st}$ denotes the existence of the match between hot stream *i* and cold stream *j* in stage *st*, the solution obtained will have at least N_{sub} subnetworks. The inequality is used in the constraint rather than the equality to allow for the solution with smaller number of matches than $N_{unit,min}$ (more number of subnetworks). However, there exist some cases wherein the minimum number of units cannot be achieved (Furman and Sahinidis, 2004). Furthermore, the solutions with the minimum number of units may not be optimal. Hence, instead of limiting the number of matches, this thesis proposes to limit the possibility of matches. The additional binary variables and corresponding constraints to enforce the solutions to have at least $N_{sub,min}$ subnetworks are as follows:

$po_{i,j}$ = 1 denotes that the match between hot stream *i* and cold stream *j* is possible
= 0 denotes that the match between hot stream *i* and cold stream *j* is not possible

Possibility to match between hot stream *i* and cold stream *j*

$$\sum_{i \in HP} \sum_{j \in CP} po_{i,j} \le N_s - N_{sub,\min} \tag{34}$$

$$\sum_{st \in ST} y_{i,j,st} - M.po_{i,j} \le 0 \qquad i \in HP, j \in CP \tag{35}$$

where *M* is a big positive number, such as number of stages (*nok*)

The additional number of binary variables $po_{i,j}$ is $N_h x N_c$. The proposed constraints can enforce the solutions to have at least $N_{sub,min}$ subnetworks. Furthermore, these constraints can also be applied to the multi-period MINLP model such as the model of Aalota (2003), and Verheyen and Zhang (2006). The modified MINLP model can be implemented for HEN synthesis with a number of subnetworks as shown in Figure 10.

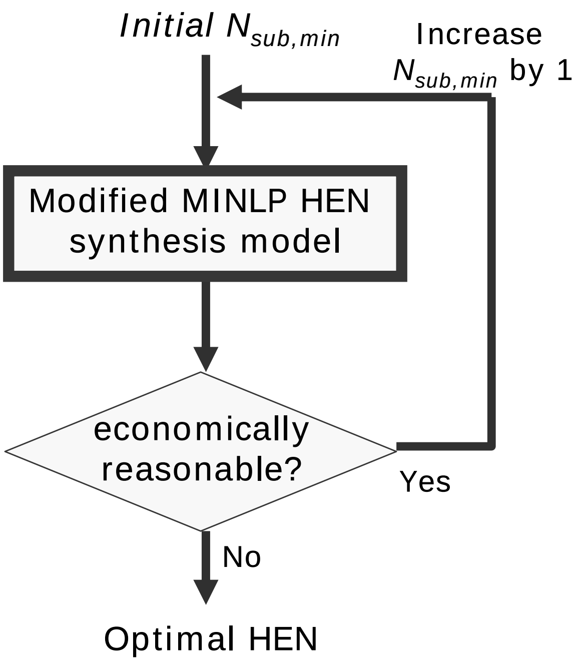


Figure 10 Implementation of the proposed modified MINLP model for HEN synthesis with a number of subnetworks

The initial value of $N_{sub,min}$ may be obtained from the solution of the original MINLP model. For a number of runs with gradually increasing the specified value of $N_{sub,min}$, the economically reasonable solution with more number of subnetworks is favorable.

RESULTS AND DISCUSSION

Part I: Optimal operation of heat exchanger networks

1. Application of the proposed approaches for determining optimal split-range control structure

1.1 Case study 1.1

The HEN from Glemmestad *et al.* (1999) as shown in Figure 11 is studied here. There are two process exchangers and two utility types ($N_U=2$). Furthermore, 4 manipulated variables, bypasses of exchangers 1 and 2 (u_{b1} and u_{b2}) and utility duties of cooler and heater (Q_c and Q_h), are available for control of all target outlet temperatures ($N_t=3$). The disturbance is ±5 ^oC in the inlet temperature of stream H1.

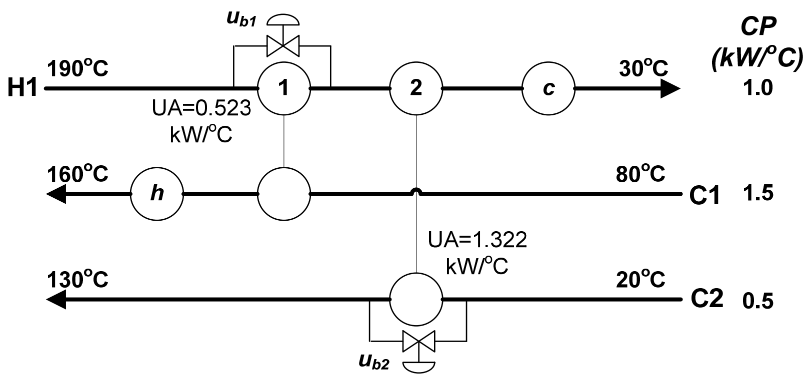


Figure 11 A simple HEN (Glemmestad *et al.*, 1999)

To see if a strategy for optimal operation is required, degrees of freedom should be first checked. The dimensional space spanned by the manipulated variables in the inner HEN to the outer HEN (*DS*) is 2. Using equation (2), we have $N_{DOF,U}$=2+2-3=1. This implies that the operation is structurally feasible. Furthermore, there is one remaining degree of freedom for utility cost optimization, hence, a strategy for optimal operation is needed.

By using approach 1 (based on the directional effect), a control structure for optimal operation of this HEN can be obtained by the following steps:

Step 1: $N_{DOF,U}$>0, hence go further to step 2.

Step 2: Solving the LP utility cost optimization problem for the nominal operating condition, the optimal solution is

Q_c(kW)	Q_h(kW)	u_{b1}	u_{b2}
67	81	0	0.02

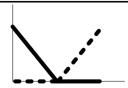
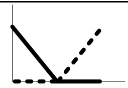
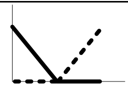
The result shows that there are three unsaturated manipulated variables (inactive constraints) for control (Q_c, Q_h and u_{b2}) and these will be assigned as primary manipulated variables. For a direct effect, the control pairing should be Q_c-T_{H1}^{out} and Q_h -T_{C1}^{out} and u_{b2}-T_{C2}^{out} . Hence, u_{b1} is the only free manipulated variable.

Step 3: The directional effect among manipulated variables and controlled variables are shown in Table 6. The information from this table is used to generate the split-range signal as shown in Table 7.

Table 6 The directional effect of manipulated variables and controlled variables in case study 1.1

Controlled variable	Primary MV			Secondary MV
	Q_c	Q_h	u_{b2}	u_{b1}
T_{H1}^{out}	−			+
T_{C1}^{out}		+		−
T_{C2}^{out}			−	+

Table 7 The split-range signal in case study 1.1

Secondary MV / Primary MV	u_{b1}	
	multiplication of sign	***Split-range signal***
Q_c	–	
Q_h	–	
u_{b2}	–	

Step 4: Table 7 shows u_{b1} can be used to protect more than one primary manipulated variable. Hence, to allow this, a selective controller is required to select a saturated signal. The resulting control structure is shown in Figure 12.

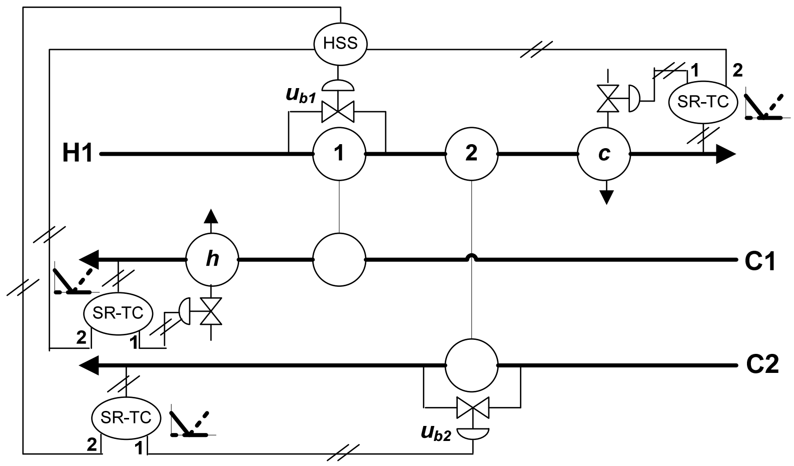


Figure 12 The resulting control structure using approach 1 in case study 1.1

Port 1 of the split-range temperature control (SR-TC) block represents the signal to the primary manipulated variable while port 2 represents the signal to the secondary manipulated variable. The high signal selective control (HSS) block is used to select the signal from port 2 of SR-TC blocks when a primary manipulated variable is saturated.

In approach 2, the additional information required is the disturbance space. In this case study, the disturbance is ±5 ^{o}C in the inlet temperature of stream H1 and this generates two active constraint regions as shown in Table 8.

Table 8 Set of active constraints in case study 1.1

Region	Manipulated variables			
	Q_c	Q_h	u_{b1}	u_{b2}
1	U	U	S_L	U
2	U	U	U	S_L

*U – Unsaturated manipulated variable (inactive constraint),

S_L – Saturated manipulated variable (active constraint) at the lower bound

Although the proposed ILP Problem P2 can be applied to propose an optimal split-range control structure, for some simple cases the solution can be obtained using an inspection. The alternately switching between u_{b1} and u_{b2} to become active constraint implies that these two manipulated variables should be combined as a split-range pair. Q_c and Q_h are never saturated, hence, they have no need for secondary manipulated variables. Assume that the region 1 is the primary region, for a direct effect the control structure should be Q_c-T_{H1}^{out}, Q_h-T_{C1}^{out} and u_{b2}-T_{C2}^{out} as shown in Figure 13.

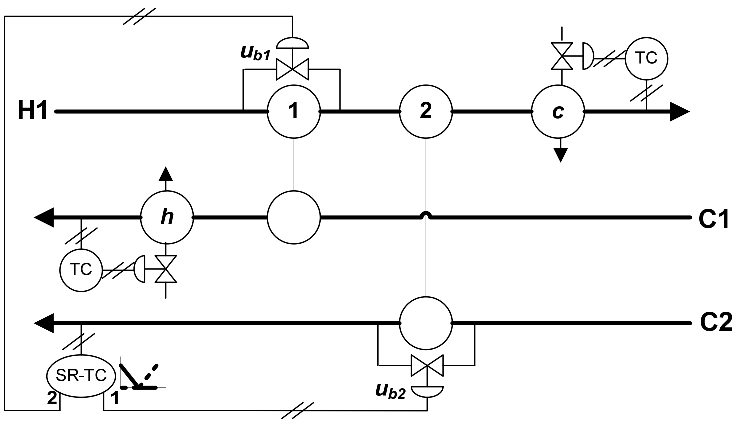


Figure 13 The resulting control structure using an inspection in case study 1.1

Split-range signal of a split-range controller can be obtained by considering the information of active constraint regions in Table 8. The split-range signal of the pair of u_{b1} and u_{b2} is  (thick line -primary manipulated variable, dash line - secondary manipulated variable) because they switch alternately to their lower constraints.

Note that the control structure obtained from approach 2 is very similar to the one obtained from approach 1 except that the complexity is reduced. This is because further information of disturbances is taken into account in the design phase. However, the control structure from the approach 1 has more flexibility and is independent of disturbances. For example, when the operation enforces Q_c to be saturated, u_{b1} can take over the task of Q_c in approach 1 while this is not possible in approach 2. Hence, the control design using approach 2 depends strongly on the information of given disturbances to generate active constraint regions.

1.2 Case study 1.2

The HEN in Figure 14 contains one hot stream and one cold stream with two target temperatures (outlet temperatures of two streams). Each process exchanger has a single bypass. This network has N_{units}=4, DS=1, N_U=2, resulting in N_{DOF}=4-2=2 and $N_{DOF,U}$=1+2-2=1.

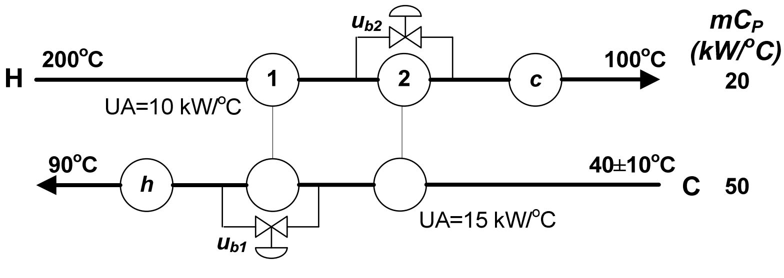


Figure 14 A simple HEN with a loop

Glemmestad (1997) showed that the number of loops (N_{loops}) can be calculated by

$$N_{loops} = N_{DOF}\text{-}N_{DOF,U} = 2\text{-}1\text{=}1 \quad (36)$$

This implies that there is one free degree of freedom that may be used for some purposes without affecting the optimum of utility cost due to the duty shift between exchangers 1 and 2. Assume that the disturbance is ±10 ^{o}C in the inlet temperature of the cold stream C (T_C^{in}).

By using approach 1, an optimal split-range control structure can be determined by the following steps:

Step 1: $N_{DOF,U}$>0, hence go further to step 2

Step 2: The solution of the LP utility cost optimization is

Q_c(kW)	Q_h(kW)	u_{b1}	u_{b2}
0	500	0.3171*	0.1966*

*multiple solutions

As expected, the LP has multiple solutions. Furthermore, the solution obtained shows the number of unsaturated manipulated variables is more than the number of target temperatures and hence the further step in this approach cannot be proceeded. However, this can be handled by choosing an appropriate constraint solution among the solution set. For a direct effect, after Q_h is chosen to control T_C^{out}, u_{b2} seems to be a better choice than u_{b1} to control T_H^{out}. In general, this solution can be found by performing a two-step optimization (i.e. lexicographic optimization) with first solving for the utility cost, and then maximizing the duty of exchanger 1 (Q_1) according to the optimal utility cost in the first step. Hence, another solution from the LP is

Q_c(kW)	Q_h(kW)	u_{b1}	u_{b2}
0	500	0	0.2424

In this new solution, the number of unsaturated manipulated variables is equal to the number of target temperatures, hence, the further step can be proceeded. Q_h and u_{b2} are assigned as primary manipulated variables for controlling T_C^{out} and T_H^{out}, respectively. The remaining manipulated variables, Q_{c1} and Q_h, are assigned as secondary manipulated variables.

Step 3: In this step, the directional effects from u_{b1} (or u_{b2}) to the two target temperatures are unclear ([±]) because of the parallel opposing effects introduced from the loop. For example, considering the effect of increasing u_{b2} to T_H^{out}, the parallel effects come from the path: exchanger 2 → exchanger 1 → exchanger 2.

When there is an unclear [±] sign, the resulting control structure from the approach 1 cannot guarantee optimality. Hence, further information from an offline optimization (i.e. active constraint regions) would be recommended. This follows approach 2.

The optimization result and active constraint regions (see the left side of Tables 9 and 10) from the LP utility cost optimization problem show that the manipulated variable Q_h (duty of the heater) is never saturated and hence Q_h has no need of a secondary manipulated variable. For the control pairing, to get a direct effect, Q_h is used to control T_C^{out} while Q_c is used to control T_H^{out}. However, because Q_c can be saturated in some operating conditions, it requires a secondary manipulated variable which may be u_{b1} or u_{b2} (bypasses of exchangers 1 or 2) or probably both. If the result on the left side of Table 10 is considered, the choice of secondary manipulated variable is not quite clear because both u_{b1} and u_{b2} are in use. However, for a direct effect, u_{b2} seems to be a better choice. This solution can be obtained by performing a two-step optimization with first solving for the utility cost, and then maximizing the duty of exchanger 1 (Q_1) according to the optimal utility cost in the first step. This results in the LP solution with 2 active constraints as shown in the right side of Tables 9 and 10.

Table 9 Optimization result of the HEN in case study 1.2

Disturbance	**Minimize utility cost (without handling multiple solutions)**				**Minimize utility cost and maximize Q_1 (with handling multiple solutions)**			
ΔT_C^{in}	u_{b1}	u_{b2}	Q_c(kW)	Q_h(kW)	u_{b1}	u_{b2}	Q_c(kW)	Q_h(kW)
0	0.3171*	0.1966*	0	500	0	0.2424	0	500
-10	0.6002*	0.3612*	0	1000	0	0.4635	0	1000
+10	0	0	48	48	0	0	48	48

*multiple optimal solutions due to duty shift between exchangers in loops

Table 10 Active constraint regions of the HEN in case study 1.2

Region	**Minimize utility cost (without handling multiple solutions)**				**Minimize utility cost and maximize Q_1 (with handling multiple solutions)**			
	u_{b1}	u_{b2}	Q_c(kW)	Q_h(kW)	u_{b1}	u_{b2}	Q_c(kW)	Q_h(kW)
1	U*	U*	S_L	U	S_L	U	S_L	U
2	S_L	S_L	U	U	S_L	S_L	U	U

U – Unsaturated manipulated variable (inactive constraint),

S_L – Saturated manipulated variable (active constraint) at the lower bound

*multiple optimal solutions

Note that the information of active constraints needed in constraint 5 of the ILP Problem P1 and P2 should be obtained from the solution in the right side of Table 10. For example, if the information of active constraints on the left side of Table 10 is used, there will be no feasible solution.

The result of active constraint regions from the solution in the right side of Table 10 shows that Q_c and u_{b2} switch alternately to become an active constraint and hence should be combined as a split-range pair. Moreover, because u_{b1} is always an active constraint, it should be assigned at the constraint for optimality. For this simple

HEN, the optimal split-range control structure can be obviously found by inspection without the need of the ILP as shown in Figure 15.

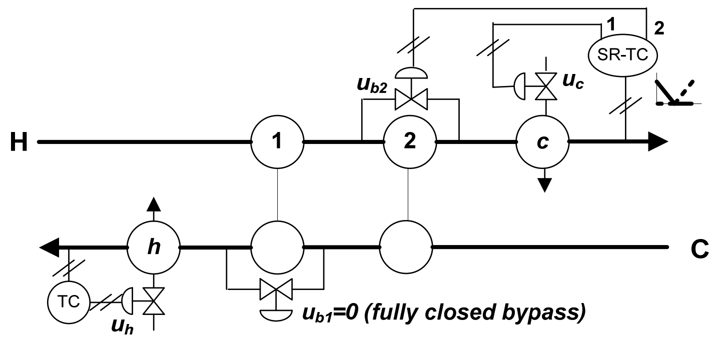


Figure 15 A trivial HEN with an optimal split-range control structure (SR-TC = split-range temperature controller)

1.3 Case study 1.3

The HEN from the work of Aguilera and Marchetti (1998) with the modification to use only single bypasses as shown in Figure 16 is studied. There are two hot and two cold process streams with target outlet temperatures. The utility prices are 0.05 \$/kW.h for hot utility h, 0.02 \$/kW.h for cold utility c1 and 0.01 \$/kW.h for cold utility c2. The disturbances are the inlet temperature of each stream, with the expected variation ±10 ^oC for streams H1, H2, and C1 and ±5 ^oC for stream C2.

Again, before moving into the design phase of control system, one should first check degrees of freedom. There are six degrees of freedom (heat duties of all exchangers) and four target outlet temperatures. This leaves two degrees of freedom for utility cost optimization ($N_{DOF,U}$=3+3-4=2).

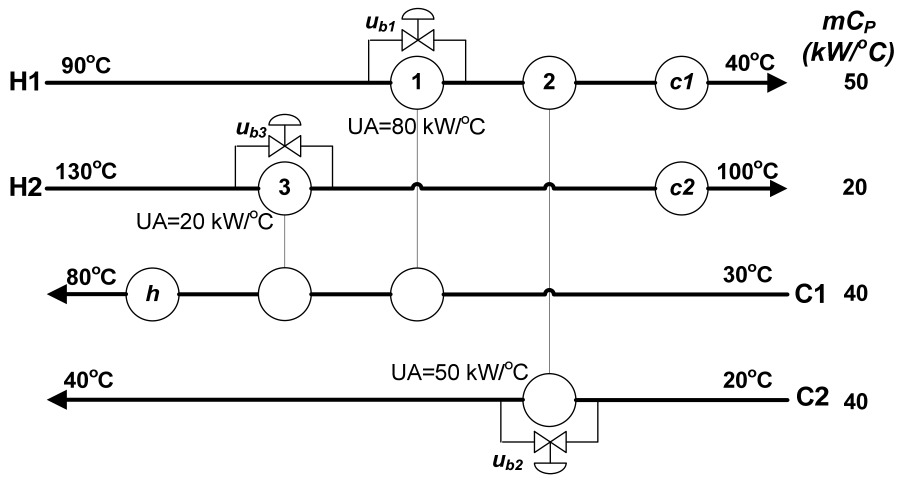


Figure 16 A HEN in case study 1.3

By using approach 1, an optimal split-range control structure can be determined by the following steps:

Step 1: $N_{DOF,U}$>0, hence go further to step 2

Step 2: The solution of the LP utility cost optimization is

Q_{c1}(kW)	Q_{c2}(kW)	Q_h(kW)	u_{b1}	u_{b2}	u_{b3}
0	300	0	0.0145	0.1463	0.7295

According to the result, Q_{c2}, u_{b1}, u_{b2} and u_{b3} will be assigned as primary manipulated variables. For a direct effect, the control pairing should be Q_{c2}-T_{H2}^{out}, u_{b1}-T_{H1}^{out}, u_{b2}-T_{C2}^{out} and u_{b3}-T_{C1}^{out}. The remaining saturated manipulated variables, Q_{c1} and Q_h, will be assigned as secondary manipulated variables.

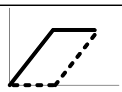
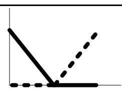
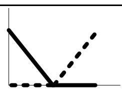
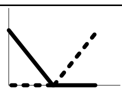
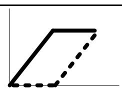
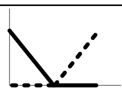
Step 3: The directional effect among manipulated variables and controlled variables are shown in Table 11. The information from this table is used to generate the split-range signal as shown in Table 12.

Table 11 The directional effect of manipulated variables and controlled variables in case study 1.3

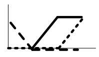
Controlled variable	**Primary MV**				**Secondary MV**	
	Q_{c2}	u_{b1}	u_{b2}	u_{b3}	Q_{c1}	Q_h
T_{H1}^{out}		+			−	0
T_{H2}^{out}	−				−*	+*
T_{C1}^{out}				−	−*	+
T_{C2}^{out}			−		+*	0

*effect from closed-loop interaction

Table 12 The split-range signal in case study 1.3

Secondary MV / **Primary MV**	Q_{c1}		Q_h	
	Multiplication of sign	**Split-range signal**	**Multiplication of sign**	**Split-range signal**
Q_{c2}	+		−	
u_{b1}	−		0	
u_{b2}	−		0	
u_{b3}	+		−	

Step 4: The result in Table 12 shows that for u_{b1} and u_{b2}, only one secondary manipulated variable (i.e. Q_{c1}) is available at the lower constraint. However, for Q_{c2} and u_{b3}, two secondary manipulated variables (i.e. Q_{c1} and Q_h) are available at both lower and upper constraints. Q_{c1} can be used at the upper constraint while Q_h can be used at the lower constraint. Note that this requires a split-range

control with three manipulated variables (such as ) resulting in a more complicated control system. The control structure is shown in Figure 17.

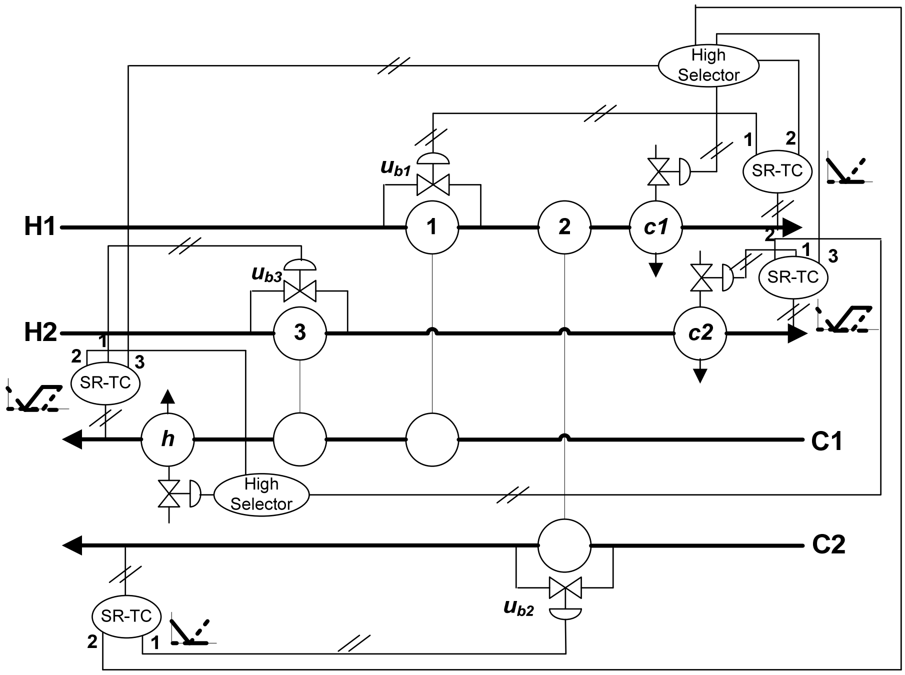


Figure 17 The resulting control structure using approach 1 in case study 1.3

In approach 2, the additional information required is the sets of active constraint regions that can be obtained using parametric programming (Kvasnica *et al.*, 2004). The resulting 5 active constraint regions are shown in Table 13.

Table 13 demonstrates that manipulated variables Q_{c1}, Q_{c2}, Q_h and u_{b1} can become active constraints at the lower bounds (i.e. zero utility duties or fully close of bypasses) while manipulated variable u_{b3} can become an active constraint at the upper bound (i.e. fully open of bypasses). The manipulated variable u_{b2} is never an active constraint (never saturated), hence, it should be used as a primary manipulated variable with no need for a secondary manipulated variable.

Table 13 Set of active constraints in case study 1.3

Region	**Manipulated variables**					
	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
1	S_L	U	S_L	U	U	U
2	S_L	S_L	U	U	U	U
3	U	S_L	U	S_L	U	U
4	U	U	S_L	S_L	U	U
5	U	U	S_L	U	U	S_U

U-Unsaturated manipulated variable (inactive constraint),
S_L-Saturated manipulated variable (active constraint) at the lower bound,
S_U-Saturated manipulated variable (active constraint) at the upper bound

For this case study, the ILP Problem P1 and P2 will be used to suggest an optimal split-range control structure. The software "GAMs" with the solver "CPLEX" was used to solve the ILP. The solution from Problem P1 (minimizing complexity in optimal split-range pairs) in Table 14 shows that Q_{c1}, Q_{c2}, u_{b1} and u_{b2} are chosen as primary manipulated variables (see diagonal elements with $x_{i,i} = 1$) while Q_h and u_{b3} are chosen as secondary manipulated variables (see diagonal elements with $x_{i,i} = 0$). Q_h is the secondary manipulated variable for Q_{c2} ($x_{2,3} = 1$) and u_{b3} is the secondary manipulated variable for Q_{c1} and u_{b1} ($x_{1,6} = 1$ and $x_{4,6} = 1$). However, the solution obtained from Problem P1 may not be unique. For example, by including the constraint $x_{3,3} = 1$ (i.e. set Q_h as a primary manipulated variable) in Problem P1, a different solution with the same value of objective function I (J_I=3) is obtained as shown in Table 15.

Table 14 The values of $x_{i,j}$ after solving Problem P1 (J_I=3)

Secondary MV / Primary MV	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
Q_{c1}	1					1
Q_{c2}		1	1			
Q_h			0			
u_{b1}				1		1
u_{b2}					1	
u_{b3}						0

(the remaining entries are zero)

Table 15 The values of $x_{i,j}$ after solving Problem P1 with setting $x_{3,3} = 1$ (J_I=3)

Secondary MV / Primary MV	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
Q_{c1}	1					1
Q_{c2}		0				
Q_h		1	1			
u_{b1}				1		1
u_{b2}					1	
u_{b3}						0

(the remaining entries are zero)

To handle the multiple solutions of Problem P1, the second objective J_{II} (controllability purpose in terms of minimizing the sum of relative orders) is introduced and included in Problem P2 for selecting the most controllable control structure. The additional information of relative orders is shown in Table 16. The values of binary variables $x_{i,j}$ and $z_{k,j}$ from solving Problem P2 are shown in Tables 17 and 18, respectively.

Table 16 Relative orders of the HEN in case study 1.3

MV / CV	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
T_{H1}^{out}	1	∞	∞	3	2	∞
T_{H2}^{out}	∞	1	∞	3	∞	2
T_{C1}^{out}	∞	∞	1	3	∞	2
T_{C1}^{out}	∞	∞	∞	2	1	∞

(the remaining entries are zero)

Table 17 The values of $x_{i,j}$ after solving Problem P2 (J_I=3)

Secondary MV / Primary MV	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
Q_{c1}	1			1		
Q_{c2}		1	1			
Q_h			0			
u_{b1}				0		
u_{b2}					1	
u_{b3}				1		1

(the remaining entries are zero)

Table 18 The values of $z_{k,j}$ after solving Problem P2 (J_{II}=5)

MV / CV	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
T_{H1}^{out}	1					
T_{H2}^{out}		1				
T_{C1}^{out}						1
T_{C2}^{out}					1	

(the remaining entries are zero)

Table 17 shows Q_{c1}, Q_{c2}, u_{b2} and u_{b3} are chosen as primary manipulated variables while Q_h and u_{b1} are chosen as secondary manipulated variables. Table 18 shows the appropriate control pairing, T_{H1}^{out}-Q_{c1}, T_{H2}^{out}-Q_{c2}, T_{C1}^{out}-u_{b3} and T_{C2}^{out}-u_{b2} (see $z_{1,1} = z_{2,2} = z_{3,6} = z_{4,5} = 1$). The resulting control structure from approach 2 is shown in Figure 18.

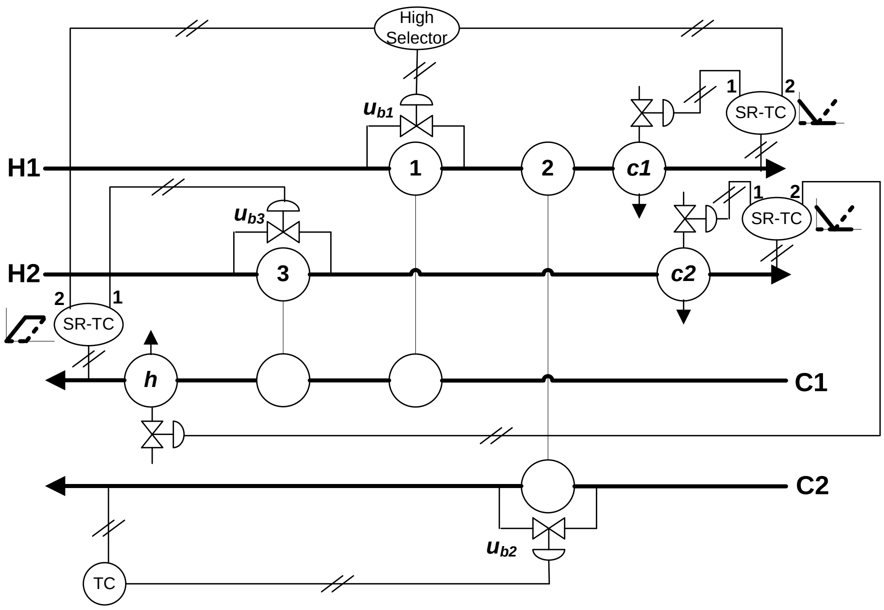


Figure 18 The resulting control structure using approach 2 in case study 1.3

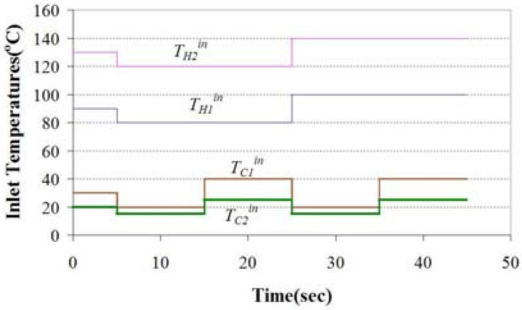
The HEN in the case study 1.3 with the resulting control structures from both approaches is tested by performing dynamic simulation on Aspen Dynamics v12.1. The information of disturbances and active constraints of the system at each period are shown in Table 19. The dynamic results show that the control structures from both approaches can provide optimality. Figure 19 shows the dynamic result of the HEN with the control structure given from approach 2. Figure 19b shows the ability of the control structure to keep all target temperatures at the desired values even under the saturation of some manipulated variables (see Figure 19d and 19e). The input saturation problem is solved by switching ability to use a secondary manipulated variable when a primary manipulated variable is saturated. Furthermore, the optimality (in terms of utility cost) is also given as shown in Figure 19c that the graph of utility cost can track the optimal line. This consequence comes from the ability of the control structure to track the right active constraint during the operation (see Figure 19d and 19e, and set of active constraints in Table 19).

Table 19 Disturbances and active constraints for each period

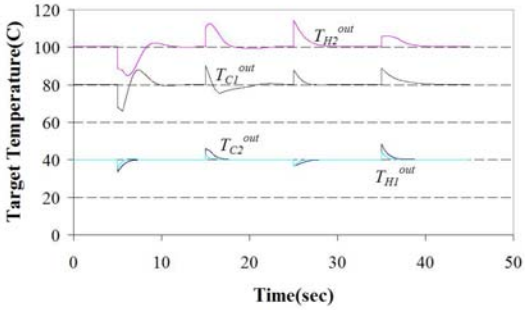
Time (sec)	**Disturbance**				**Active constraint**					
	ΔT_{H1}^{in}	ΔT_{H2}^{in}	ΔT_{C1}^{in}	ΔT_{C2}^{in}	Q_{c1}	Q_{c2}	Q_h	u_{b1}	u_{b2}	u_{b3}
less than 5	0	0	0	0	S_L		S_L			
5-15	-10	-10	-10	-5	S_L	S_L				
15-25	-10	-10	10	5		S_L		S_L		
25-35	10	10	-10	-5	S_L		S_L			
more than 35	10	10	10	5			S_L			S_U

S_L-Saturated manipulated variable (active constraint) at the lower bound,

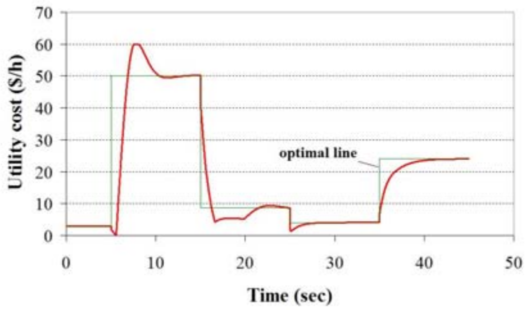
S_U-Saturated manipulated variable (active constraint) at the upper bound



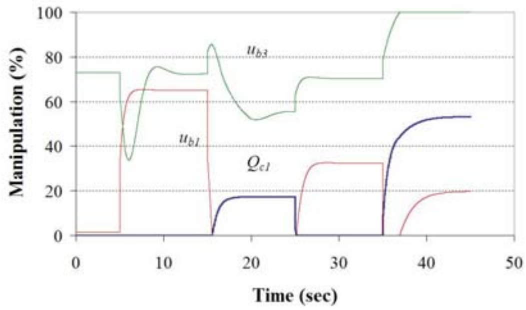
(a) Inlet temperatures



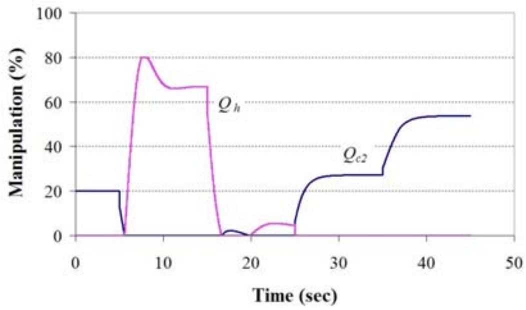
(b) Target temperatures



(c) Utility cost



(d) Manipulated variable (Q_{c1}, u_{b1} and u_{b3})



(e) Manipulated variable (Q_{c2} and Q_h)

Figure 19 Dynamic simulation of the HEN in case study 1.3 with the resulting control structures from approach 2

Part II: HEN synthesis with controllability improvement

2. Application of the proposed structural controllability evaluation tool

2.1 Case study 2.1: Selection of a control structure

In this case study, the ILP Problem P3 is used to propose a potential control structure of the HEN in Figure 4. Relative orders ($r_{k,j}$) and the possibility of having parallel opposing effects ($p_{k,j}$) that are required in the optimization are shown in Tables 20 and 21.

Table 20 $r_{k,j}$ of the HEN in case study 2.1

	Q_1	Q_2	Q_3	Q_4
T_{H1}	2	1	3	∞
T_{H2}	∞	∞	1	1
T_{C1}	1	2	2	∞

Table 21 $p_{k,j}$ of the HEN in case study 2.1

	Q_1	Q_2	Q_3	Q_4
T_{H1}	1	1	1	0
T_{H2}	0	0	0	0
T_{C1}	1	1	1	0

Additional information required in the optimization is the sets of manipulated variables for SISO control systems with structural singularity (MVS^n). The ranks in Table 4 show that the set {Q_1, Q_2, Q_3} and {Q_1, Q_2, Q_4} should be avoided. Hence, the equations of constraint 4 in Problem P3 are,

$$\sum_{k \in CV} z_{k,1} + \sum_{k \in CV} z_{k,2} + \sum_{k \in CV} z_{k,3} \leq 2 \qquad (37)$$

$$\sum_{k\in CV} z_{k,1} + \sum_{k\in CV} z_{k,2} + \sum_{k\in CV} z_{k,4} \leq 2 \qquad (38)$$

If the preference order of objective functions is assumed as *RO*, N_{POE}, and *DI*, respectively, then the proposed control pairs are T_{H1}-Q_2, T_{H2}-Q_4, and T_{C1}-Q_3 ($z_{1,2}=1$, $z_{2,4}=1$ and $z_{3,3}=1$ as shown in Table 22). The resulting structural indicators are *RO*=4, N_{POE}=2, and *DI*=2.33. The implication of *RO*=4 (that is greater than the number of controlled variables) is that some control pairs cannot have direct effects. This can be illustrated from the matrix of $[r_{k,j}]\otimes[z_{k,j}]$, where ⊗ denotes element by element multiplication. Table 23 shows that the relative order of the pair T_{C1}-Q_3 is 2.

Table 22 $z_{k,j}$ of the HEN in case study 2.1

	Q_1	Q_2	Q_3	Q_4
T_{H1}	0	1	0	0
T_{H2}	0	0	0	1
T_{C1}	0	0	1	0

Table 23 $[r_{k,j}]\otimes[z_{k,j}]$ in case study 2.1

	Q_1	Q_2	Q_3	Q_4
T_{H1}		1		
T_{H2}				1
T_{C1}			2	

Table 24 $[p_{k,j}]\otimes[z_{k,j}]$ in case study 2.1

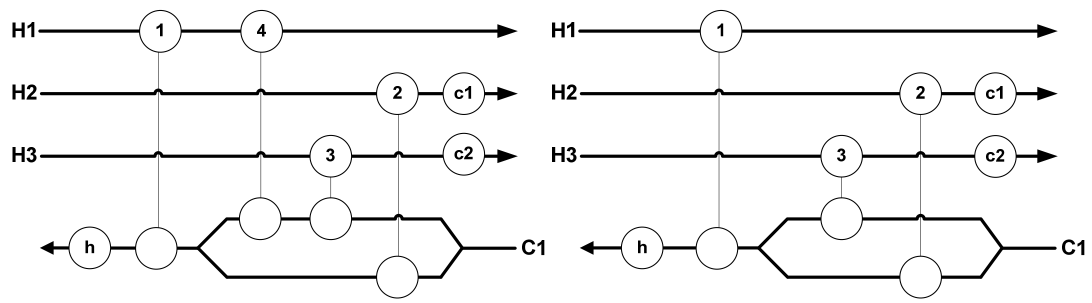
	Q_1	Q_2	Q_3	Q_4
T_{H1}		1		
T_{H2}				0
T_{C1}			1	

N_{POE}=2 implies that there are two control loops with parallel opposing effects. The matrix $[p_{k,j}]\otimes[z_{k,j}]$ in Table 24 shows that the control loop, T_{H1}-Q_2 and T_{C1}-Q_3 may introduce RHP-zeros. *DI*=2.33 implies that the control system has some coupling effects.

Note that the above result is based on the preference order of the objectives as *RO*, N_{POE}, and *DI*, respectively. If the preference order is changed, a different solution may be given. However, for this network, the same solution is still proposed for the other preference orders. Hence, in the structural point of view, the best potential control pairing is T_{H1}-Q_2, T_{H2}-Q_4, and T_{C1}-Q_3.

2.2 Case study 2.2: Comparison among HEN structure alternatives

This case study shows the application of the proposed structural analysis for selecting the more controllable HEN structure. Two alternatives of HEN structures, HEN#1 and HEN#2, were synthesized by sequential and simultaneous designs taken from Biegler *et al.* (1997) as shown in Figure 20.



(a) HEN#1 synthesized using sequential design

(b) HEN#2 synthesized using simultaneous design

Figure 20 Two possible HEN structures

Assume that the target temperatures are the outlet temperatures of all streams and the preference order in objective function is *RO*, N_{POE}, and *DI*, respectively. The optimal solutions are addressed with *RO*=4, N_{POE}=1, and *DI*=0.33 for HEN#1 and *RO*=4, N_{POE}=0, and *DI*=0.5 for HEN#2. Both networks have identical value of *RO* and *RO*=4 implies that a direct effect is possible. However, RHP-zeros may occur in the control system of HEN#1 (N_{POE}=1) whereas it does not for HEN#2 (N_{POE}=0). Based on the possibility to have RHP-zeros, HEN#2 is more controllable. Although HEN#1 (*DI*=0.33) tends to be more structurally decoupled than HEN#2 (*DI*=0.5), the interaction is considered to be less important.

In addition, HEN#1 was further analyzed by changing the preference order of the objectives. The results show that even though N_{POE} is rearranged as the primary objective, the control system of HEN#1 still exhibits some parallel opposing effects (with N_{POE}=1). This confirms that HEN#1 has some deficiency compared to HEN#2. The structural difference between HEN#1 and HEN#2 is the existence of the heat exchanger 4 in HEN#1. Although the use of the duty of exchanger 4 as a manipulated variable for the outlet temperature of stream H1 of HEN#1 can reduce the off-diagonal relative order corresponding to the outlet temperature of stream C1, it introduces a heat load loop that can cause parallel opposing effects. This example demonstrates that the use of only relative orders and decoupling index for structural analysis (e.g. Lee *et al.*, 2001) may mislead to a poor HEN structure. Supplementary of RHP-zeros analysis should be included in the structural controllability analysis of a process.

3. The application of the proposed MINLP HEN synthesis model with specified number of subnetworks

3.1 Case study 3.1: Single-period model

In this case study, the proposed MINLP model will be applied to a single-period HEN synthesis problem. Stream information is shown in Table 25.

Table 25 Stream information for case study 3.1

Stream	Inlet temperature (^oC)	Outlet temperature (^oC)	Heat capacity flowrate ($kW/^oC$)
H1	85	45	156.3
H2	120	40	50
H3	125	35	23.9
H4	56	46	1250
H5	90	85	1500
H6	225	74	50
C1	40	55	466.7
C2	55	65	600
C3	65	165	195
C4	10	170	81.3

The other information used here are:

individual heat transfer coefficients for all streams = 0.05 $kW/m^{2o}C$
steam cost = 100 \$/kW/yr
cooling water cost 15 \$/kW/yr
unit cost = 6000 \$/unit
area cost = 600 $\$/m^2$
lifetime used = 6 years, and rate of interest = 3%

For this case study, the original model of Yee and Grossman (1990) was first run a number of times to find an appropriate value of minimum allowable temperature difference (DT_{min}) and maximum allowable hot utility (HU_{up}) available (Aalota, 2003; Verheyen and Zhang, 2006). The number of stages used here is 3. The software "GAMs" was used to solve the optimization problem on AMD Turion64 MT30 with Ram 512 MB. The solvers used were "DICOPT" for MINLP, "MINOS" for NLP and "CPLEX" for MIP.

Table 26 shows that the best objective value can be found by DT_{min} = 10 ^{o}C and HU_{up} = 35,000 kW, hence, these values will be used for the remaining optimizations in the case study.

Table 26 Results from the original model with different values of DT_{min} and HU_{up}

DT_{min} (^{o}C)	HU_{up} (kW)	TAC ($)	DT_{min} (^{o}C)	HU_{up} (kW)	TAC ($)
5	35,000	9,860,865	15	35,000	9,806,310
	30,000	9,860,865		30,000	9,663,942
	25,000	9,860,865		25,000	9,605,088
	20,000	10,060,248		20,000	Infeasible
10	**35,000**	**9,451,469**	20	35,000	10,054,170
	30,000	9,474,666		30,000	10,054,170
	25,000	9,474,666		25,000	Infeasible
	20,000	9,836,640		20,000	Infeasible

Considering the solution obtained by using DT_{min} = 10 ^{o}C and HU_{up} = 35,000 kW, there are 3 subnetworks. Hence, to look for the solution with more number of subnetworks (>3), the first try should be the search for the solution with 4 subnetworks.

To have the solution with at least 4 subnetworks, one may try to limit the upper bound of the number of matches by 6 ($N_{unit,min}$ = N_s-N_{sub} = 10-4 = 6) and add the corresponding constraint, $\sum_i \sum_j \sum_{st} y_{i,j,k} \leq N_{unit,\min}$ into the model of Yee and Grossman (1990). This model will be referred as “Model A”. The solution from the problem has TAC = $9,526,094. However, limiting the number of matches to the minimum reduces the solution space and the global solution may be cut off. This problem can be avoided by using the proposed MINLP model. By assigning $N_{sub,min}$ = 4, the solution obtained has TAC = $9,515,254 with 7 matches. This shows the advantage of the proposed model that allows for the solution with more than minimum number of matches. Refer to the resulting solutions, increasing the number of subnetworks from 3 to 4 increases $63,785 or 0.67% in terms of total annual cost.

The search for solutions with more number of subnetworks was run a number of times, with varying the upper bound of $N_{unit,min}$ in Model A and varying $N_{sub,min}$ in the proposed model. The results were shown in Table 27.

Table 27 Comparison of the solutions obtained from the model of Yee and Grossman (1990) with limiting the upper bound of the number of matches, and the proposed model.

Model A				**Proposed model**				
$N_{sub,min}$	**TAC ($)**	N_{sub}	**CPU Time (s)**	$N_{sub,min}$	**TAC ($)**	N_{sub}	N_{unit}	**CPU Time (s)**
-	9,451,469	3	0.93					
4	9,526,094	4	3.1	4	9,515,254	4	7	8.69
5	9,582,039	5	1.95	5	9,543,429	5	6	21.32
6	9,618,365	6	1.09	6	9,618,365	6	4	4.34
7	9,674,501	7	1.28	7	10,300,123	7	3	4.59
8	10,183,459	8	0.46	8	10,356,259	8	2	1.88
9	Infeasible*	-	-	9	Infeasible*	-	-	-

*the infeasibility caused by the limit of HU_{up}

For the solutions with 4 and 5 subnetworks, the proposed model can provide better solutions than Model A in terms of total annual cost. However, for the solution with 6 subnetworks, both models can provide the same values of TAC. For the solution with 7 and 8 subnetworks, the proposed model provides worse solutions than model A that contrast to one's intuition. This problem comes from a large pool of local optima because of the nonconvexity of the MINLP model. Furthermore, the additional binary variables in the proposed model increase the difficulty in solution searching. Using the proposed model with $N_{sub,min} = 7$, the solver was trapped at the solution with TAC = \$10,300,123 whereas using Model A with $N_{unit,min}$ = 3, the solution has TAC = \$9,674,501. Hence, for some cases, the proposed model may not provide a better solution comparing to Model A if the solver was trapped at some worse local optima.

Considering the computational time, as expected the proposed model requires more CPU time because of the difficulty introduced by the additional binary variables. However, with the increase of computer speed, this seems to be a minor problem.

3.2 Case study 3.2: Multi-period model

The HEN synthesis problem in this case study comes from Aalota (2003) with the modification to consider the area cost of utilities. Stream information is shown in Table 28. The heat capacity flowrate of stream H2 is considered as an uncertain parameter in the rage of 1-1.18 kW/^{o}C.

Table 28 Stream information for case study 3.2

Stream	Period 1			Period 2		
	Inlet temperature (^{o}C)	**Outlet temperature (^{o}C)**	**Heat capacity flowrate (kW/^{o}C)**	**Inlet temperature (^{o}C)**	**Outlet temperature (^{o}C)**	**Heat capacity flowrate (kW/^{o}C)**
H1	450	280	2	450	280	2
H2	310	50	1	310	50	1.8
C1	115	290	2	115	290	2
C2	40	120	3	40	120	3

The other information used here are:

individual heat transfer coefficients for all streams = 8 kW/m^{2o}C steam cost = 115.2 €/kW/yr

cooling water cost = 1.3 €/kW/yr

unit cost = 8333.3 €/unit

area cost = 641.7 €/m^2

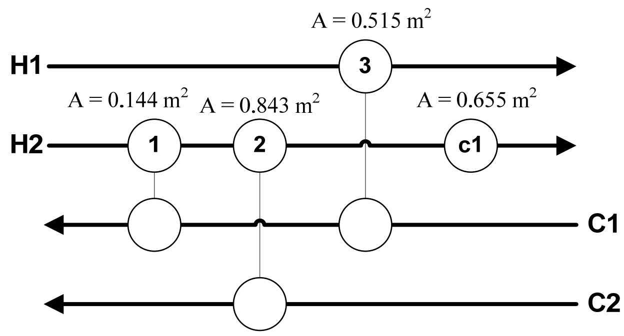
lifetime used = 3 years and rate of interest= 18%

In this case, the proposed constraint equations will be applied into the multi-period MINLP model of Aalota (2003). The minimum allowable approach temperature (DT_{min}) used here is 10 ^{o}C and the upper bound of the hot utility duty has no limit. Furthermore, the number of stages is 3 and stream splitting is not allowed. The solvers used were “DICOPT” for MINLP, “MINOS” for NLP and “CPLEX” for MIP.

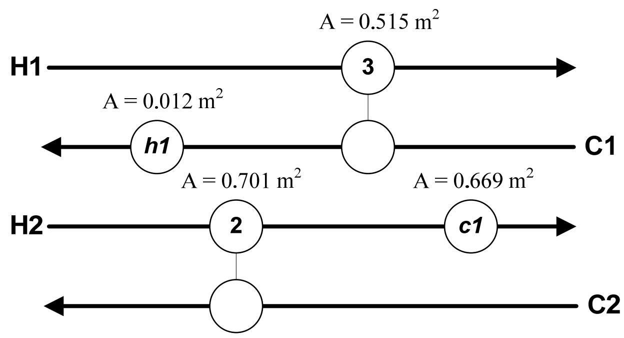
The results obtained from the original model of Aalota (2003) and the modified model with varying $N_{sub,min}$ are summarized in Table 29. Increasing the number of subnetworks from 1 to 2 increases €1,106 or 5.8% in terms of total annual cost. However, to have 3 or 4 subnetworks, one has to additionally pay €29,043 (or 153%) and €68,661 (or 362%), respectively, that were totally unacceptable. The solutions with 1 and 2 subnetworks are shown in Figure 21.

Table 29 Results from the proposed model with different values of $N_{sub,min}$

Model	**TAC (€)**	N_{sub}
Aalota model (2003)	18,975	1
Modified Aalota model with $N_{sub,min}$ =2	20,081	2
Modified Aalota model with $N_{sub,min}$ =3	48,018	3
Modified Aalota model with $N_{sub,min}$ =4	87,636	4



(a) solution with 1 subnetworks



(b) solution with 2 subnetworks

Figure 21 The resulting HEN structures in case study 3.2

CONCLUSION AND RECOMMENDATION

Conclusion

Two issues on HENs were addressed in this thesis. The first issue concerns optimal operation of HENs. The outcome of this is the design methodologies of optimal split-range control structures. The second issue concerns controllability improvement in HEN synthesis. The outcomes are (i) a structural controllability evaluation tool, and (ii) a HEN synthesis technique with a number of subnetworks.

Part I: Optimal operation of heat exchanger networks

For certain HENs that only single bypasses and utility duties are considered as manipulated variables, optimal operation problem of HENs can be formulated as a linear program (LP). This LP formulation implies that optimal solutions will always lie at some input constraint vertices. However, under the variation of operating condition, the optimal active constraints may change and this motivates a need for a control policy with the ability to optimally switch between active constraint regions. The suggestion is to use a simple split-range control scheme that is probably the easiest way to implement the optimal switching. Two approaches to design an optimal split-range control structure were proposed.

In approach 1, the information from the LP utility cost optimization at a specified nominal period is firstly used to determine primary manipulated variables for control pairings, and then the information of directional effect among manipulated variables and controlled variables will be used to generate optimal split-range pairs. The advantage of the first approach is that the resulting control structure is independent of disturbances, hence, has more flexibility. When the information of disturbances is limited, approach 1 would be suggested. However, this is compensated with a more complicated control structure, especially for a large HEN problem. Furthermore, the optimality cannot be guaranteed in case some directional effects are unclear. Hence, to handle these disadvantages, additional information of disturbance spaces would be suggested and this follows approach 2.

In approach 2, the information of active constraint regions in a given disturbance window and relative orders are used in the proposed integer linear program (ILP) Problems P1 and P2 to determine an optimal split-range control structure. Nevertheless, for a small HEN problem with a small number of active constraint regions, an optimal split-range control structure may be simply found using one's intuitive inspection. The advantage of approach 2 is that the complexity of the control structure can be reduced (the first objective in the proposed ILP) comparing to approach 1. However, the flexibility given by the control system will depend upon the given disturbance window in the design phase. Furthermore, in the proposed ILP formulation, only two manipulated variables are allowed in a split-range pair, whereas in practice more than two manipulated variables in a split-range pair may be possible.

It is possible for some HENs to have no optimal split-range control structure such as no feasible solution of the ILP Problems P1 and P2. Hence, a study on a technique for switching between active constraint regions should be further investigated. The technique is expected to be applicable for not only constraint (vertex) optimal operation problem, but also unconstraint (non-vertex) optimal operation problem (e.g., simplifying an online optimization task).

Part II: HENs synthesis with controllability improvement

Heat integration can be obtained by using heat exchanger networks. However, the integration may introduce some difficulties for control. Hence, the issue of controllability should not be overlooked in the process design. This work focuses on structural controllability improvement in the HEN synthesis. Two methods to improve structural controllability were proposed.

The first method is based on the sequential approach, that is, among the economically reasonable solution set of HEN structure alternatives obtained from a number of synthesis techniques, the structure with the best structural controllability evaluation is more favorable. The structural criteria used are structural singularities, parallel opposing effects, relative orders, and decoupling indices, in which the evaluation is formulated as the ILP Problem P3. To solve Problem P3, the preference order of the three objectives in Problem P3 needs to be first chosen. A change of the preference order may result to a different solution. In general, the order of RO, N_{POE}, and DI, is suggested.

The second method to improve controllability in HEN synthesis is to search for an economically reasonable solution with a number of subnetworks. The availability of subnetworks in HENs presents a number of advantages including operability and controllability issues (Shethna and Jezowski, 2006). The MINLP model of Yee and Grossman (1990) is improved by introducing binary variables and corresponding constriants to enforce the solutions to have at least user-specified number of subnetworks. From a number of runs with different values of user-specified number of subnetworks, the economically reasonable solution with more number of subnetworks is favorable. One problem found when solving the problem is a trap of local optima. This consequence comes from the inherent nonconvexity in the original MINLP model. Furthermore, the increase of the binary variables in the proposed model additionally introduces some more difficulties in searching for the solution of DICOPT. Hence, solving the proposed model with another MINLP solver such as SBB should be further investigated. SBB may perform better than DICOPT for the problem with more difficult nonlinearities (GAMs Development Corp., 2002).

Recommendation

Part I: Optimal operation of heat exchanger networks

1. The proposed ILP for determining optimal control structure allows only two manipulated variables in a split-range combination. Hence, the development of a more complex ILP with allowing more manipulated variables in a split-range combination should be further investigated.

2. The proposed approaches to determine optimal split-range control structure is not hopefully applicable for HENs only, but also for the processes that optimal operation is always at a constraint vertex. The implementation of optimal split-range control structure to other processes would be interesting.

3. In this thesis, only the constraint optimal operation problem of HENs is considered. For the unconstraint optimal operation problem such as when split fractions or multi-bypasses are allowed as manipulated variables, the research on this problem such as a simple strategy with avoiding an online optimization to implement the optimal operation would be challenging to be investigated.

Part II: HENs synthesis with controllability improvement

1. The proposed technique for structural controllability evaluation is hopefully applicable for other processes. The application of the proposed method to other processes should be further investigated.

2. The only available MINLP solver for using in this thesis is DICOPT. Hence, solving the proposed modified MINLP problem with another MINLP solver such as SBB may provide more insight on the solutions.

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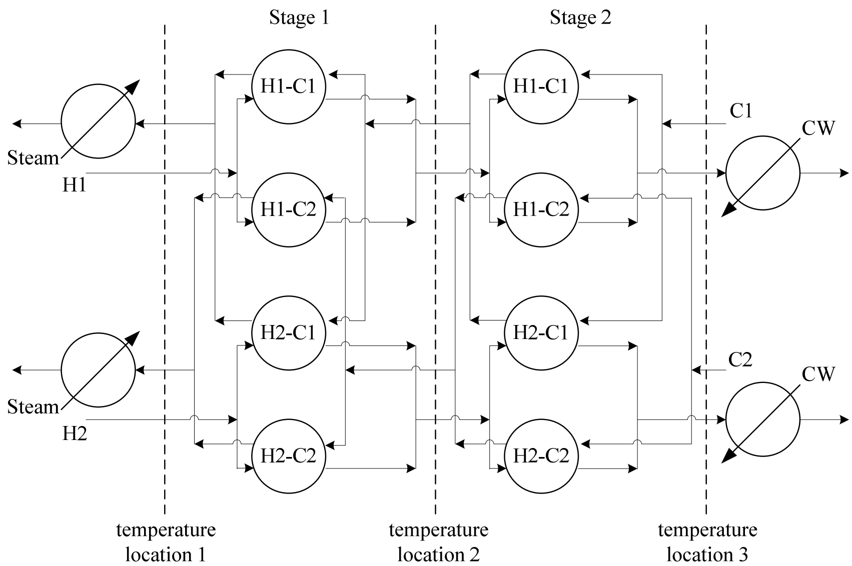
APPENDIX

Simultaneous MINLP synthesis model for heat exchanger networks

Yee et al. (1990) proposed the stage-wise superstructure for the presentation of potential matches among hot and cold streams. A superstructure example for two hot and two cold streams is shown in Appendix Figure 1.



Appendix Figure 1 Stage-wise superstructure

Based on this idea, Yee and Grossman (1990) proposed a MINLP formulation for HEN synthesis. Definitions of parameters and variables used in the formulation are:

Sets

HP	=	set of hot process streams
CP	=	set of cold process streams
ST	=	set of superstructure stages

Parameters

TIN_i	=	inlet temperature of stream i (^oC)

$TOUT_i$	=	outlet temperature of stream *i* (^oC)
$(mC_p)_i$	=	heat capacity flow rate of stream *i* ($kW/^oC$)
$U_{i,j}$	=	overall heat transfer coefficient of hot stream i and cold stream *j* ($kW/^oC.m^2$)
Ucu_i	=	overall heat transfer coefficient correspond to cold utility exchanger of hot stream *i* ($kW/^oC.m^2$)
Uhu_j	=	overall heat transfer coefficient correspond to cold utility exchanger of cold stream *j* ($kW/^oC.m^2$)
Ccu	=	unit cost for cold utility (kW/$)
Chu	=	unit cost for hot utility (kW/$)
β	=	exponent for area cost
nok	=	total number of stages
Q_{up}	=	upper bound for heat exchanged (kW)
AF	=	annual factor
$CF_{i,j}$	=	fixed charge for match of hot stream *i* and cold stream *j* ($/unit)
$CFcu_i$	=	fixed charge for cold utility exchanger of hot stream *i* ($/unit)
$CFhu_j$	=	fixed charge for hot utility exchanger of cold stream *j* ($/unit)
$CA_{i,j}$	=	area cost coefficient for match of hot steam *i* and cold stream *j* ($\$/m^2$)
$CAcu_i$	=	area cost coefficient for cold utility exchanger of hot stream *i* ($\$/m^2$)
$CAhu_j$	=	area cost coefficient for hot utility exchanger of cold stream *j* ($\$/m^2$)
DT_{min}	=	minimum allowable temperature difference (^oC)
DT_{up}	=	maximum allowable temperature difference (oC)
HU_{up}	=	maximum allowable hot utility (kW)

Variables

$dt_{i,j,st}$	=	temperature difference for match of hot stream *i* and cold stream *j* at stage *st* (^oC)

$dtcu_i$ = temperature difference for match of hot stream *i* and cold utility (^{o}C)

$dthu_j$ = temperature difference for match of cold stream *j* and hot utility (^{o}C)

$q_{i,j,st}$ = heat exchanged between hot stream *i* and cold stream *j* at stage *st* (kW)

qcu_i = heat exchanged between hot stream *i* and cold utility (kW)

qhu_j = heat exchanged between cold stream *j* and hot utility (kW)

$t_{i,st}$ = temperature of hot stream *i* at hot end of stage *st* (^{o}C)

$t_{j,st}$ = temperature of cold stream *j* at cold end of stage *st* (oC)

Binary variables

$y_{i,j,st}$ = existence of match of hot stream *i* and cold stream *j* at stage *st*

ycu_i = existence of cold utility exchanger for hot stream *i*

yhu_j = existence of hot utility exchanger for cold stream *j*

With the above definitions of parameters and variables, the MINLP formulation for HEN synthesis can now be presented,

$$\begin{aligned}
\text{min TAC} = \; & AF.\left[\sum_{i\in HP}\sum_{j\in CP}\sum_{st\in ST} CF_{i,j}.y_{i,j,st} + \sum_{i\in HP} CFcu_i.ycu_i + \sum_{j\in CP} CFhu_j yhu_j\right] \\
& + AF.\sum_{i\in HP}\sum_{j\in CP}\sum_{st\in ST} CA_{i,j}\left[\frac{q_{i,j,st}}{U_{i,j} LMTD_{i,j,st}}\right]^{\beta} \\
& + AF.\sum_{j\in CP} CAhu_j\left[\frac{qhu_j}{Uhu_j LMTDhu_j}\right]^{\beta} \\
& + AF.\sum_{i\in HP} CAcu_i\left[\frac{qcu_i}{Ucu_i LMTDcu_i}\right]^{\beta} \\
& + \sum_{i\in HP} Ccu.qcu_i + \sum_{j\in CP} Chu.qhu_j \qquad \text{(A1)}
\end{aligned}$$

Subject to:

Overall heat balance for each stream

$$(TIN_i - TOUT_i)(mC_p)_i = \sum_{st \in ST} \sum_{j \in CP} q_{i,j,st} + qcu_i \qquad i \in HP \qquad \text{(A2)}$$

$$(TOUT_j - TIN_j)(mC_p)_j = \sum_{st \in ST} \sum_{i \in HP} q_{i,j,st} + qhu_j \qquad j \in CP \qquad \text{(A3)}$$

Heat balance at each stage

$$(t_{i,st} - t_{i,st+1})(mC_p)_i = \sum_{j \in CP} q_{i,j,st} \qquad i \in HP, st \in ST \qquad \text{(A4)}$$

$$(t_{j,st} - t_{j,st+1})(mC_p)_j = \sum_{i \in HP} q_{i,j,st} \qquad j \in CP, st \in ST \qquad \text{(A5)}$$

Assignment of superstructure inlet temperatures

$$TIN_i = t_{i,1} \qquad i \in HP \qquad \text{(A6)}$$

$$TIN_j = t_{j,nok+1} \qquad j \in CP \qquad \text{(A7)}$$

Feasibility of temperatures

$$t_{i,st} \geq t_{i,st+1} \qquad i \in HP, st \in ST \qquad \text{(A8)}$$

$$t_{j,k} \geq t_{j,st+1} \qquad j \in CP, st \in ST \qquad \text{(A9)}$$

$$TOUT_i \leq t_{i,nok+1} \qquad i \in HP \qquad \text{(A10)}$$

$$TOUT_j \geq t_{j,1} \qquad j \in CP \qquad \text{(A11)}$$

Hot and cold utility duty

$$(t_{i,nok+1} - TOUT_i)(mC_p)_i = qcu_i \qquad i \in HP \qquad \text{(A12)}$$

$$(TOUT_j - t_{j,1})(mC_p)_j = qhu_j \qquad j \in CP \qquad \text{(A13)}$$

Logical constraints

$$q_{i,j,st} - Q_{up} y_{i,j,st} \leq 0 \qquad i \in HP, j \in CP, st \in ST \qquad \text{(A14)}$$

$$qcu_i - Q_{up} ycu_i \leq 0 \qquad i \in HP \qquad \text{(A15)}$$

$$qhu_j - Q_{up} yhu_j \leq 0 \qquad j \in CP \qquad \text{(A16)}$$

Calculation of approach temperatures

$$dt_{i,j,st} \leq t_{i,st} - t_{j,st} + DT_{up}(1 - y_{i,j,st}) \qquad i \in HP, j \in CP, st \in ST \qquad \text{(A17)}$$

$$dt_{i,j,st+1} \leq t_{i,st+1} - t_{j,st+1} + DT_{up}(1 - y_{i,j,st}) \qquad i \in HP, j \in CP, st \in ST \qquad \text{(A18)}$$

$$dtcu_i \leq t_{i,nok+1} - TOUT_{cu} + DT_{up}(1 - ycu_i) \qquad i \in HP \qquad \text{(A19)}$$

$$dthu_j \leq TOUT_{hu} + DT_{up}(1 - yhu_j) \qquad j \in CP \qquad \text{(A20)}$$

$$dt_{i,j,st} \geq DT_{\min} \qquad i \in HP, j \in CP, st \in ST \qquad \text{(A21)}$$

Total hot utility availability (Aalota, 2003)

$$\sum_{j \in CP} qhu_j \leq HU_{up} \qquad j \in CP \qquad \text{(A22)}$$