See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/231376554

# Systematic Optimization of Heat-Integrated Water Allocation Networks

ARTICLE in INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · APRIL 2011

Impact Factor: 2.59 · DOI: 10.1021/ie1016392

**CITATIONS READS** 

22

46

# 4 AUTHORS, INCLUDING:



Zuwei Liao

**Zhejiang University** 

48 PUBLICATIONS 412 CITATIONS

SEE PROFILE



**Gang Rong** 

**Zhejiang University** 

98 PUBLICATIONS 678 CITATIONS

SEE PROFILE



**Yongrong Yang** 

**Zhejiang University** 

92 PUBLICATIONS 605 CITATIONS

SEE PROFILE





# Systematic Optimization of Heat-Integrated Water Allocation Networks

Zuwei Liao, \*, \* Gang Rong, \*, \* Jingdai Wang, \*, \* and Yongrong Yang \*

ABSTRACT: This paper deals with the design of heat integrated water utilization networks. The nonisothermal mixing and freely splitting nature of hot and cold streams have made the problem far more complicated than the design of heat exchanger networks (HEN). By establishing an MILP model, promising heat exchange matches between hot and cold streams are obtained first without considering the detailed network design. Subsequently, a stage-wise HEN superstructure is introduced for the detailed network design. The proposed systematic approach can be applied for large scale problems. Examples from literature and a practical example in a PVC plant are used to illustrate the applicability of the approach.

# 1. INTRODUCTION

Energy and water are important resources to process industries. Since modern society faces energy shortage and water scarcity problems, much attention has been paid to reduce energy and water consumption. Consequently, considerable techniques have been developed for the optimization of water allocation networks (WAN) and heat exchanger networks (HEN). These techniques are mainly based on conceptual design or mathematical programming. Comprehensive reviews of WAN can be found in Bagajewicz, <sup>1</sup> Foo, <sup>2</sup> and Jezowiski, <sup>3</sup> while comprehensive reviews of HEN can be found in Linnhoff, <sup>4</sup> Furman and Sahinidis. <sup>5</sup>

In process industries, water is a carrier of both contaminants and energy. Therefore, water utilization and energy consumption should be considered simultaneously. The combined consideration has gained benefits in water networks of pulp industries<sup>o,/</sup> and refineries.8 However, despite all those improvements in WAN and HEN, the study of integrated water allocation and heat exchange networks (abbreviated as WAHEN) has only initiated in recent years. Savulscu and Smith<sup>9-11</sup> introduced a conceptual approach which involves a two-stage procedure. In the first stage, a twodimensional grid diagram is developed to explore different options for minimum water and energy consumption. In the second stage, the concept of a separate system is adopted to simplify the heat exchange networks (HEN) design. Subsequently, other conceptual design tools such as source-demand energy composite curves, <sup>12</sup> graphical thermodynamic rule <sup>13</sup>, heat surplus diagrams, <sup>7</sup> and water energy balance diagrams 14 were developed to evaluate direct heat transfer and simplify the design of HEN. In addition, recent conceptual developments also include rules for both negligible contaminant <sup>15</sup> and multicontaminant cases. <sup>16,17</sup>

Mathematical programming techniques have also been used for the problem. These techniques combined the models of WAN and HEN together. Bagajewicz et al. <sup>18</sup> applied a state—space representation for the combined WAN and HEN. In the same work, they introduced a superstructure model for the WAN, and employed a transhipment model for the HEN. Both linear programming (LP) and mixed integer linear programming

(MILP) models were generated to obtain the utility targets and the detailed network, respectively. Later, this transhipment formulation of HEN was modified for distinguishing the direct and indirect heat transfer, 19 and then extended to consider operation split.<sup>20</sup> Subsequently, several superstructure-based HEN representations have been introduced for simultaneous optimization. Leewongtanawit and Kim<sup>21</sup> combined the transhipment model with a hyper-structure model,<sup>22</sup> and Bogataj and Bagajewicz<sup>23</sup> modified a stage-wise superstructure to represent the HEN in the WAHEN. These two models used heuristics to constrain the number of hot and cold streams in the HEN. Although such decisions have been justified by the reduced size of the model, potential promising network structures might be excluded from the stream-selecting heuristics. On the other hand, Dong and Chang et al. 24,25 introduced a superstructure model in the HEN of the state-space representation.<sup>18</sup> This model captures much richer network structures, but is very large in size and causes an extremely heavy computational burden when the problem scale increases. At these points, it is necessary to reconsider the sequential methods not only for solving problems of larger scale but also for selecting hot and cold streams more reasonably.

In this paper, a step-wise systematic procedure is presented for the synthesis of WAHEN. The proposed procedure first specifies hot and cold streams, and then steps of targeting and design will be followed. In the targeting step, the promising matches between hot and cold streams are identified by an MILP model. The proposed MILP problem involves an extended transshipment model that treats the direct heat transfer and the indirect heat transfer separately. In the design step, a stage-wise superstructure is extended to deal with the splitting and nonisothermal mixing features inside the HEN. The design problem is formulated as an MINLP problem. The advantage of the proposed

Received: August 1, 2010
Accepted: February 22, 2011
Revised: February 15, 2011
Published: April 20, 2011

<sup>†</sup>State Key Laboratory of Industrial Control Technology, Zhejiang University, Hangzhou, 310027, Zhejiang, China

<sup>&</sup>lt;sup>‡</sup>State Key Laboratory of Chemical Engineering, Department of Chemical Engineering and Biochemical Engineering, Zhejiang University, Hangzhou 310027, Zhejiang, China

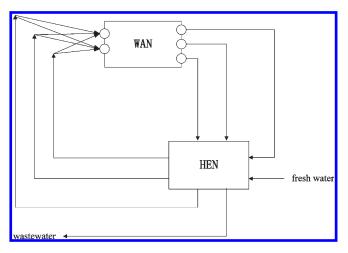
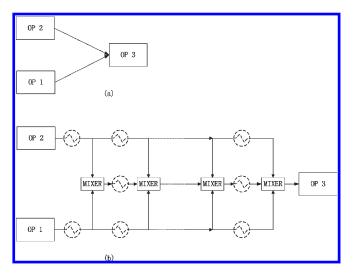


Figure 1. Representation of WAHEN.



**Figure 2.** (a) Flow pattern of two-stream mix; (b) possible flow patterns of two-stream mixing considering temperature constraints.

method is illustrated via examples from literature and an industrial case study, a PVC plant.

#### 2. PROBLEM STATEMENT

The problem addressed in this paper can be stated as follows: A set of water-using processes *P* that require water of a certain quality and temperature is given. The freshwater source is specified with given contaminant concentration and temperature while the discharge streams are specified to be below a maximum temperature. The objective then is to derive a water stream distribution network and a HEN between these streams that minimizes the total cost.

The basic assumptions that are made to this synthesis problem are that for the water-using processes the maximum inlet and outlet concentrations of contaminant, contaminant mass load, and operating temperature are specified at constant value. In addition, to concentrate on the energy and networks structure features of the WAHEN, single contaminant operations are assumed, and the system is assumed to be operating continuously.

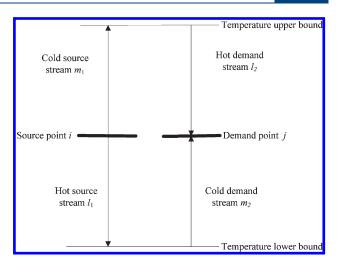


Figure 3. Definition of hot and cold streams.

The general framework of WAHEN can be represented by Figure 1. The WAHEN is composed of two interconnected blocks: the WAN and the HEN. The water-using operations are presented in the WAN block, while all the heat-exchanger units are presented in the HEN. Before building any of the mathematical models, let us identify the hot and cold streams first.

#### 3. IDENTIFICATION OF HOT AND COLD STREAMS

In the traditional HEN model, hot and cold streams are recognized as having constant flow rate and explicit starting and ending temperatures. However, when splitting and mixing happens, such definition may not be applicable. Take two streams mixing as an example. If we do not consider the temperature constraints, the flow pattern of mixing is simply shown as Figure 2a. If temperature constraints are considered, then possible flow patterns are represented as Figure 2b. In Figure 2b there are many streams whose starting and ending temperatures are uncertain. Therefore, it is difficult to tell whether it is hot stream or cold stream. Besides, if we put all these streams into the HEN model, the problem can be combinatorially demanding. To identify hot and cold streams and control the number of them, we specify the hot/cold streams in a new way in this section.

Consider the streams from source point *i*, as shown in Figure 3. Before these streams achieve any of the demand points, their temperature change is assumed either monotone decrease or monotone increase. The temperature monotone decreasing stream from source point i is designated as hot source stream (HS) and denoted by  $l_1$ , while the temperature monotone increasing stream from source point *i* is designated as cold source stream (CS) and denoted by  $m_1$ . Similarly, consider the streams that flow to demand point j. After they leave any of the source points, their temperature changes are also assumed either monotone decrease or monotone increase. The temperature monotone decreasing stream to demand point *j* is designated as hot demand stream (HD) and denoted by  $l_2$ , while the temperature monotone increasing stream to demand point *j* is designated as cold demand stream (CD) and denoted by  $m_2$ . All the HS and HD form the set of hot streams, while all the CS and CD form the set of cold streams. The whole system has temperature upper and lower bounds which correspond to the highest and lowest temperatures among the freshwater, wastewater, and operation

units. The ending temperatures of the source streams and the starting temperatures of the demand streams are fixed to the system temperature bound. Note that the flow rate of the streams is changing, since stream mixing and splitting happens. From the above definition, there are two hot and two cold possible streams for one process unit, and the upper bound of total number is  $2N_{\rm p}+N_{\rm ww}+N_{\rm w}$  for hot or cold streams, where  $N_{\rm p},N_{\rm ww}$ , and  $N_{\rm w}$  are the number of process units, wastewater treatment units, and freshwater resources, respectively. On the other hand, since freshwater is not allowed to mix with waste streams before discharge in this article, the number of possible connections in the WAN is calculated as  $(N_{\rm p}+N_{\rm ww}+N_{\rm w})\times N_{\rm p}$ . Therefore, the number of hot and cold streams is constrained to a relative small value. In summary, the number of hot and cold streams can be identified before any calculation.

Now, let us take an example from Savulescu et al. <sup>11</sup> to see how the hot and cold streams are identified. This example consists of four water-using process units whose operating parameters are presented in Table 1. The upper bound of the hot/cold stream number is calculated as 10. In addition, the wastewater discharge temperatures are specified at 30 °C. Because only the temperature of freshwater is below this 30 °C, there are no cold stream flow to the wastewater treatment units. On the other hand, since the temperature of fresh water and operation two are at the lowest and highest extreme, respectively, there is no hot stream flow from fresh water or flow to operation 2, and no cold stream flow from operation 2. Consequently, eight hot and eight cold streams can be identified, as shown in Figure 4. In Figure 4, the solid lines with arrow denote source streams, while the dotted lines with arrow represent demand streams. Specially, the

Table 1. Data for Example 1<sup>a</sup>

process number	mass load of contaminant $(g/s)$	C <sub>in</sub> <sup>max</sup> (ppm)	C <sub>out</sub> <sup>max</sup> (ppm)	temperature (°C)
1	2	0	100	40
2	5	50	100	100
3	30	50	800	75
4	4	400	800	50

<sup>&</sup>lt;sup>a</sup> Temperature of fresh water  $T_{\rm w}$  = 20°C; temperature of wastewater  $T_{\rm out}$  = 30°C.

streams with arrow point down are hot streams; otherwise, they are cold streams. With the specified hot and cold streams, we will extend the transshipment model of HEN in next section to find the design targets.

#### 4. MATHEMATICAL MODEL

The HEN in the WAHEN is much more complicated than the traditional one, not only because the streams are allowed to mix and split freely, but also because the mixing can be either isothermal or nonisothermal. The existence of nonisothermal mixing may help reduce the number of heat exchangers, but on the other hand, the nonlinear nature of nonisothermal mixing will increase the computational burden. Moreover, when combining such an effect with a large number of streams which incurs the combinatorial complexity, the problem is very difficult to solve. To avoid such computational difficulty while obtaining competitive results, we decompose the problem into two steps: targeting and design. The targeting step screens promising binary combinations by omitting nonlinear items. Then, the design step optimizes the WAHEN using nonlinear model, since the combinatorial space is reduced by the previous step.

4.1. Stream Match Targeting. In this section, we will determine the heat exchange matches between hot and cold streams without considering the detailed HEN design. A modified transshipment model is introduced to represent the HEN. The transshipment model is based on the previous identified hot and cold streams. Apart from the traditional HEN transshipment model,<sup>27</sup> the modified version only allows flow mixing between hot streams and between cold streams, respectively. Such mixing has two possibilities: isothermal mixing and nonisothermal mixing. Nonisothermal mixing between streams may cause  $\Delta T_{\rm min}$  contradiction in the indrect heat transfer inside the transshipment model. Furthermore, the nonisothermal mixing cannot improve the energy target, because direct heat transfer between hot stream and cold stream is not allowed in the transshipment model. Therefore, we specify that only isothermal mixing happens inside the transshipment model. On the other hand, outside the HEN the stream mixing is treated nonisothermally when hot stream mixed with cold stream. The interactions between HEN and WAN in the stream match targeting stage is shown in Figure 5.

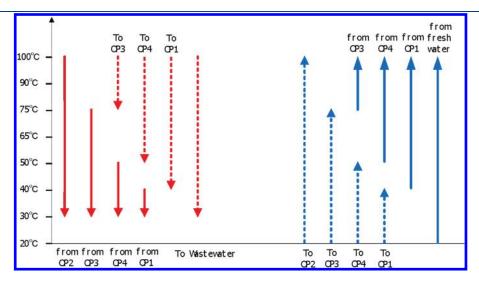


Figure 4. Hot and cold stream identification of example 1.

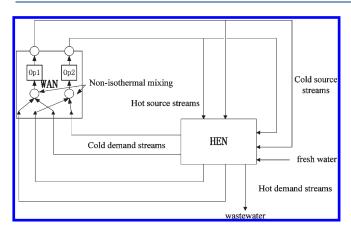


Figure 5. WAN and HEN interaction scheme in the targeting stage.

4.1.1. Flow Pattern Description. Let us consider the flow regime between streams inside the HEN. Since the temperature change of these streams are assumed monotone, then water flow transfer between a hot stream and a cold stream is not allowed within the HEN. Therefore, water flow transfer between streams happens either from HS to HD, or from CS to CD. To ensure the temperature difference of heat transfer, the temperature of hot streams are shifted by subtracting the minimum temperature approach  $\Delta T_{\min}$ . The whole HEN temperature range can be divided into several temperature levels which correspond to the starting and ending temperature of hot and cold streams. The isothermal mixings are specified at these temperature levels, while the indirect heat exchange happens at the intermediate temperature intervals. Figure 6 panels a and b illustrate the case between  $l_1$ ,  $l_2$  and  $m_1$ ,  $m_2$ , respectively. Hot source stream  $l_1$  flows from source point i to the corresponding temperature level and then to hot demand stream  $l_2$  in this temperature level with the remainder going to adjacent lower temperature levels. Cold source stream  $m_1$  flows from source point i to the corresponding temperature level and then to cold demand stream  $m_2$  in this temperature level with the remainder going to adjacent lower temperature levels. The highest temperature level is denoted by k= 1, while the lowest level is denoted by k = K + 1. Figure 7 shows the flow pattern of different mixers and splitters at temperature level k. Since the starting and ending temperature levels are unique for each stream, the numbers of splitters/mixers are not the same between streams.

According to Figure 6 and Figure 7, one can write down the following mass balance equations for each mixer and splitter:

$$fh_{l_{2},k} = fh_{l_{2},k-1} + \sum_{l_{1} \in HT_{l_{2}}} trh_{l_{1},l_{2},k} \quad \forall l_{2} \in HD, k \leq k_{l_{2}^{k}}$$

$$fh_{l_{1},k} = fh_{l_{1},k-1} - \sum_{l_{2} \in HT_{l_{1}}} trh_{l_{1},l_{2},k} \quad \forall l_{1} \in HS, k \geq k_{l_{1}^{k}}$$

$$(2)$$

$$fc_{m_2,k} = fc_{m_2,k-1} + \sum_{m_1 \in CT_{m_2}} trc_{m_1,m_2,k} \quad \forall m_2 \in CD, k \ge k_{m_2^{\epsilon}}$$
(3)

$$fc_{m_1,k} = fc_{m_1,k-1} - \sum_{m_2 \in CT_{m_1}} trc_{m_1,m_2,k} \quad \forall m_1 \in CS, k \leq k_{m_1^s}$$
(4)

$$\begin{array}{l} fh_{l_2,1}, fh_{l_1,K+1}, fc_{m_2,K+1}, fc_{m_1,1} \\ = 0 \quad \forall \ l_2 \in HD, \ l_1 \in HS, \ m_2 \in CD, \ m_1 \in CS \end{array} \ \ (5)$$

4.1.2. Transshipment Model of HEN. Let us consider the heat exchange inside each temperature interval. In this section we extend the transshipment model of Papoulias and Grossmann,<sup>27</sup> which is based on temperature interval partitioning, to represent the heat exchange. Figure 8 illustrates the heat flow pattern in each temperature interval. The main modification we made on the original model is that the temperatures of streams leaving the HEN are not fixed, because nonisothermal mixing between hot and cold streams may happen outside the HEN.

Energy balance at each temperature interval:

$$rqh_{l,k+1} - rqh_{l,k} + qc_{l,k} + \sum_{m \in C_k} q_{l,m,k}$$

$$= fh_{l,k}(to_k - to_{k+1})cp \quad l \in H, k_l^* \le k \le k_l^*$$
(6)

$$\operatorname{rqc}_{m,k} - \operatorname{rqc}_{m,k+1} + \operatorname{qh}_{m,k} + \sum_{l \in H_k} q_{l,m,k}$$

= 
$$fc_{m,k}(to_k - to_{k+1})cp$$
  $m \in C, k_{m^e} \le k \le k_{m^s}$  (7)

$$rqh_{l,k_{le}} = 0 \quad l \in HS \tag{8}$$

$$rqc_{m,k,m^e} = 0 \quad m \in CS \tag{9}$$

Energy balance at the inlet of process units:

$$rqc_{m, k_{m^e}} = rqh_{l, k_{l^e}} \quad l \in HD, m \in CD, l^e = m^e$$
  
=  $j, j \in D$  (10)

Logical constraints:

$$\sum_{k=\max(k_F,k_{m^e})}^{\min(k_F,k_{m^s})} q_{l,m,k} - \Omega zsd_{l,m} \leq 0 \quad l \in H, m \in C$$
 (11)

$$\sum_{k=k_{m^{\epsilon}}}^{k_{m^{\epsilon}}} \mathrm{qh}_{m,k} - \Omega z \mathrm{h}_{m} \leq 0 \quad m \in C$$
 (12)

$$\sum_{k=k_{ls}}^{k_{le}} qc_{l,k} - \Omega zc_{l} \le 0 \quad l \in H$$
 (13)

$$zsd_{l,m}, zh_m, zc_l = 0, 1$$
 (14)

where the binary variables  $zsd_{l,m}$ ,  $zh_m$ , and  $zc_l$  count the number of matches between hot and cold streams.

4.1.3. Mathematical Model of WAN. To constrain the problem of the targeting stage to an MILP problem, a linearlized model is adopted for the WAN. The mathematical formulation is from Savelski and Bagajewicz, <sup>26</sup> they eliminated the nonlinear items by setting the outlet concentrations to their maximum values. Although this linearization is not a necessary optimal condition for simultaneous minimizing of both freshwater and energy, it retains the targeting stage in a linear problem which is efficient to solve. The formulation of the problem is as follows:

Inlet and outlet mass balance of each operation:

$$fi_i = fj, \quad i = j, j \in P \tag{15}$$

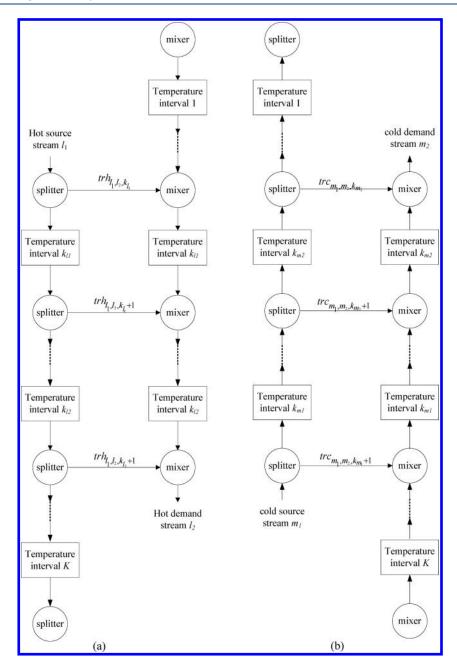


Figure 6. (a) Flow pattern between HS and HD; (b) flow pattern between CS and CD.

Contaminant mass balance of each operation:

$$\sum_{i \in \hat{P}} f_{i,j} (C_{i,\text{out}}^{\text{max}} - C_{j,\text{out}}^{\text{max}}) + L_j = 0 \quad j \in P$$
 (16)

Maximum inlet concentration constraint:

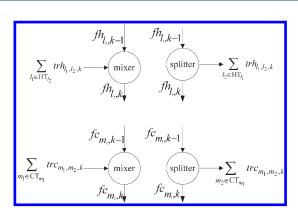
$$\sum_{i \in \hat{P}} f_{i,j} \left( C_{i,\text{ out}}^{\text{max}} - C_{j,\text{ in}}^{\text{max}} \right) \le 0 \quad j \in P$$
 (17)

Mass balance at the inlet of each operation:

$$fj_j = \sum_{i \in \hat{P}} f_{i,j} \quad j \in P$$
 (18)

Mass balance at the outlet of each operation:

$$fi_{i} = \sum_{j \in \tilde{P}f_{i,j} \quad i \in P}$$
 (19)



**Figure 7.** Flow pattern in each mixer and splitter between temperature interval k-1 and k.

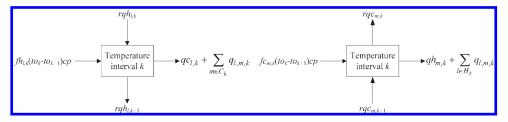


Figure 8. Heat flow pattern of hot and cold streams in temperature interval k.

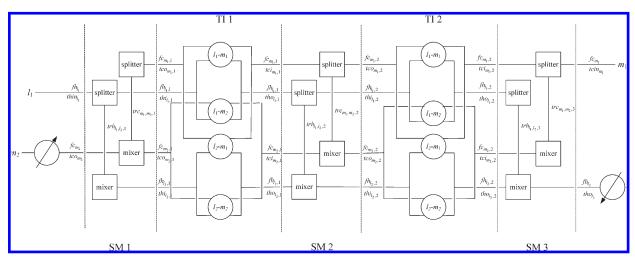


Figure 9. Heat exchanger network superstructure.

Equations 15-19 are mass balances for water material and contaminant. According to eqs 15-19, this model is linear. Consequently, the number of variables will be reduced as suggested by the necessary condition.

In addition, the connections between WAN and HEN can be represented as follows:

$$f_{l_1, l_2} = f_{i,j} \quad \forall l_1^s = i, l_2^e = j, (i,j) \in HP$$
 (20)

$$f_{m_1, m_2} = f_{i,j} \quad \forall m_1^s = i, m_2^e = j, (i,j) \in CP$$
 (21)

$$f_{m_1, m_2} = f_{i,j} \quad \forall \quad m_1^s = i, \quad m_2^e = j, (i, j) \in \text{CP}$$

$$f_{l_1, l_2} = \sum_{k = k_{l_1}^s} \text{trh}(l_1, l_2, k) \quad \forall \quad (l_1, l_2) \in \text{HT}$$
(22)

$$f_{m_1, m_2} = \sum_{k=k_{m_1^c}}^{k_{m_1^c}} \operatorname{trc}(m_1, m_2, k) \quad \forall (m_1, m_2) \in \operatorname{CT}$$
 (23)

4.1.4. Objective Function. The aim is to minimize the sum of the annualized capital costs and the utility costs that are incurred during operating. The minimum number of heat exchange matches usually corresponds to a minimum or near minimum capital cost. In this stage we roughly estimate the cost of heat exchange matches by experience. Therefore, the number of matches and the utility consumption are presented in the object function. The problem of targeting can then be formulated as the following MILP problem:

$$\begin{aligned} & \min \text{ CFW} \sum_{i \in P} f_{w,i} + \text{CCU} \sum_{m \in \text{ CU}} \text{qc}_m + \text{CHU} \sum_{l \in \text{ HU}} \text{qh}_l \\ & + \text{CFF} (\sum_{l \in H} \sum_{m \in C} \text{zsd}_{l,m} + \sum_{m \in C} \text{zh}_m + \sum_{l \in H} \text{zc}_l) \end{aligned} \tag{P1}$$

subject to eqs 1-23 where CFW, CCU, CHU, and CFF are cost coefficients for freshwater, cold utility, hot utility, and heat

Table 2. Cost and Operating Parameters of Example 1 Case a

parameter		parameter		parameter	
CCU CHU	150 \$/kw 260 \$/kw		50,000 \$ 3000 \$	tcui tcuo	10 °C 20 °C
CFW	2.5 \$/t	h (process	$1 \text{ kw/(m}^2 \text{ °C)}$	thui	126 °C
		stream and cold utility)			
CF	10000 \$	h (hot utility)	$5 \text{ kw/(m}^2  ^{\circ}\text{C})$	thuo	126 °C
CO	860 \$	В	0.75	$\Delta T_{\rm min}$	10 °C

exchange matches. It should be noted that the number of heat exchange matches do not equal the number heat exchangers. As we will see in the case studies, one match might be achieved by more than one heat exchanger. Therefore, superstructure-based approaches are needed to implement the targeted heat exchange matches.

**4.2. WAHEN Design.** 4.2.1. HEN Superstructure Representation. To carry out the detailed HEN design, we present a superstructure of the HEN in this section. The stage-wise superstructure developed by Yee and Grossmann<sup>28</sup> is extended for considering stream splitting and mixing. In the extended superstructure, the match schemes between hot and cold streams are determined by the previous step. Figure 9 shows a 2-hot-2cold stream illustration of the modified stage-wise superstructure. In this figure, the four streams are in different types, they are HS, HD, and CS, CD, respectively. Note that Figure 9 illustrates all possible match schemes between the hot and cold streams, while in practice the match schemes should be in consistence with the results of the targeting step. The whole superstructure is divided into two sections by the dashed lines: the temperature interval (TI) and the splitting/mixing section (SM), and they turn out one after another. The water flow patterns inside the TI are the same as the original superstructure. Since it is well-known, the basic feature of TI is not repeated here. Let us concentrate on the stream mixing and splitting patterns in SM. The water flow patterns inside the mixers and splitters of SM are similar to those shown in Figure 6: water flows from HS to HD, and from CS to CD via the mixers and splitters. But there are two main differences between these two water flow patterns. The first one is that the inlet and outlet temperature of each mixer/splitter are not fixed in this superstructure model. The second one is that the maximum number of mixers and splitters are identical for each hot and cold stream, and they are K+1. This is because the nonisothermal option enlarges the range of mixing.

The mathematical model is composed of WAN model, HEN model, and the connections between them. The WAN model is the same as those in section 3. The HEN model includes submodels of SM and TI. Let us consider these submodels in the following sections.

4.2.2. Model of SM Section. Mass balance at the mixers for HD and CD streams:

$$\label{eq:fhli_2,k} fh_{l_2,\,k} = \begin{cases} fh_{l_2,\,k-1} + \sum_{l_1 \, \in \, \operatorname{HT}_{l_2}} \operatorname{trh}_{l_1,\,l_2,\,k} & k = \, 2, ..., K \\ \\ \sum_{l_1 \, \in \, \operatorname{HT}_{l_2}} \operatorname{trh}_{l_1,\,l_2,\,l} & k = \, 1 \end{cases} \qquad \forall \,\, l_2 \, \in \, \operatorname{HM} \, \cap \, \operatorname{HD},$$

$$\mathsf{fh}_{l_2} = \mathsf{fh}_{l_2,K} + \sum_{l_1 \in \mathsf{HT}_{l_2}} \mathsf{trh}_{l_1,\,l_2,K+1} \quad \forall \ l_2 \in \mathsf{HM} \cap \mathsf{HD}$$

$$fc_{m_{2},k} = \begin{cases} fc_{m_{2},k+1} + \sum_{m_{1} \in CS} trc_{m_{1},m_{2},k+1} & k = 1,2,...,K-1 \\ \sum_{m_{1} \in CT_{m_{2}}} trc_{m_{1},m_{2},K+1} & k = K \end{cases}$$

$$\forall m_{2} \in CM \cap CD$$
 (26)

$$fc_{m_2} = fc_{m_2, 1} + \sum_{m_1 \in CT_{m_2}} trc_{m_1, m_2, 1} \quad \forall m_2 \in CM \cap CD$$
(27)

Mass balance at the splitters for HS and CS streams:

$$\mathrm{fh}_{l_1,k} = \begin{cases} \mathrm{fh}_{l_1,k-1} - \sum_{l_2 \in \mathrm{HD} \, \cap \, \mathrm{HM}} \mathrm{trh}_{l_1,l_2,k} & k = 2,...,K \\ \mathrm{fh}_{l_1} - \sum_{l_2 \in \mathrm{HT}_{l_1}} \mathrm{trh}_{l_1,l_2,1} & k = 1 \\ & \forall \, l_1 \in \mathrm{HM} \, \cap \, \mathrm{HS} \end{cases} \tag{28}$$

$$fh_{l_1,K} = \sum_{l_2 \in HT_{l_1}} trh_{l_1,l_2,K+1} \quad \forall l_1 \in HM \cap HS \quad (29)$$

$$fc_{m_1,k} = \begin{cases} fc_{m_1,k+1} - \sum_{m_2 \in CT_{m_1}} trc_{m_1,m_2,k+1} & k = 1,2,...,K-1 \\ fc_{m_1} - \sum_{m_2 \in CT_{m_1}} trc_{m_1,m_2,K+1} & k = K \end{cases}$$

$$m_1 \in CM \cap CS$$
(30)

$$fc_{m_1,1} = \sum_{m_2 \in CT_{m_1}} trc_{m_1,m_2,1} \quad m_1 \in CM \cap CS$$
 (31)

Energy balance at the mixers of each interval for HD and CD streams:

$$\begin{split} & \text{fh}_{l_{2},k} \times \text{thi}_{l_{2},k} \times \text{cp} \\ & = \begin{cases} & \text{fh}_{l_{2},k-1} \times \text{tho}_{l_{2},k-1} \times \text{cp} \\ & + (\sum_{l_{1} \in \text{HN} \, \cap \, \text{HT}_{l_{2}}} (\text{trh}_{l_{1},l_{2},k} \times \text{thin}_{l_{1}}) \\ & + \sum_{l_{1} \in \text{HM} \, \cap \, \text{HT}_{l_{2}}} (\text{trh}_{l_{1},l_{2},k} \times \text{tho}_{l_{1},k-1})) \\ & \times \text{cp} \quad k = 2, ..., K \\ & (\sum_{l_{1} \in \, (\text{HN} \, \cup \, \text{HM}) \, \cap \, \text{HT}_{l_{2}}} (\text{trh}_{l_{1},l_{2},1} \times \text{thin}_{l_{1}})) \times \text{cp} \quad k = 1 \\ & \forall \, l_{2} \in \, \text{HM} \, \cap \, \text{HD} \end{cases} \end{split}$$

$$\begin{split} fh_{l_{2}} \times tho_{l_{2}} \times cp &= fh_{l_{2},K} \times tho_{l_{2},K} \times cp \\ &+ \big(\sum_{l_{1} \in HN \cap HT_{l_{2}}} (trh_{l_{1},l_{2},K+1} \times thin_{l_{1}}) \\ &+ \sum_{l_{1} \in HM \cap HT_{l_{2}}} (trh_{l_{1},l_{2},K+1} \times tho_{l_{1},K}) \big) \times cp \\ &\forall \ l_{2} \in HM \cap HD \\ &fc_{m_{2},k} \times tci_{m_{2},k} \times cp = \end{split}$$

$$\begin{cases} fc_{m_{2},k+1} \times tco_{m_{2},k+1} \times cp \\ + \left(\sum_{m_{1} \in CN \cap CT_{m_{2}}} (trc_{m_{1},m_{2},k+1} \times tcin_{m_{1}}) \\ + \sum_{m_{1} \in CM \cap CT_{m_{2}}} (trc_{m_{1},m_{2},k+1} \times tco_{m_{1},k+1}) \right) \\ \times cp \quad k = 1,...,K-1 \\ \sum_{m_{1} \in (CM \cup CN) \cap CT_{m_{2}}} (trc_{m_{1},m_{2},k+1} \times tcin_{m_{1}}) \times cp \quad k = K \end{cases}$$

$$\forall m_{2} \in CM \cap CD \qquad (34)$$

$$fc_{m_{2}} \times tco_{m_{2}} \times cp = fc_{m_{2},1} \times tco_{m_{2},1} \times cp$$

$$+ \left( \sum_{m_{1} \in CN \cap CT_{m_{2}}} (trc_{m_{1},m_{2},1} \times tcin_{m_{1}}) \right)$$

$$+ \sum_{m_{1} \in CM \cap CT_{m_{2}}} (trc_{m_{1},m_{2},1} \times tco_{m_{1},1}) \times cp$$

$$\forall m_{2} \in CM \cap CD$$

$$(35)$$

Energy balance at the splitters for HS and CS streams:

$$thi_{l_1,k} = \begin{cases} tho_{l_1,k-1} & k = 2,...,K \\ thin_{l_1} & k = 1 \end{cases} \quad \forall \ l_1 \in HM \cap HS \quad (36)$$

$$tci_{m_1,k} = \begin{cases} tco_{m_1,k+1} & k = 1, 2, ..., K-1 \\ tcin_{m_1} & k = K \end{cases} m_1 \in CM \cap CS$$
(37)

4.2.3. Model of TI Section. Heat balance at each interval:

$$fh_{l,k} \times (thi_{l,k} - tho_{l,k}) \times cp$$

$$= \sum_{m \in CM} q_{l,m,k} \quad l \in HM, \ k = 1, 2, ..., K$$
(38)

$$fc_{m,k} \times (tco_{m,k} - tci_{m,k}) \times cp$$

$$= \sum_{l \in HM} q_{l,m,k} \quad m \in CM, k = 1, 2, ..., K$$
(39)

Approach temperature constraints:

$$\begin{aligned} \text{dth}_{l,m,k} &\leq \text{tho}_{l,k} - \text{tci}_{m,k} + \Gamma \\ &\times (1 - z_{l,m,k}) \quad (l,m) \in \text{MA}, \\ &k = 1, 2, ..., K \end{aligned} \tag{40}$$

$$\begin{aligned}
dtc_{l, m, k} &\leq thi_{l, k} - tco_{m, k} + \Gamma \\
&\times (1 - z_{l, m, k}) \quad (l, m) \in MA, \\
k &= 1, 2, ..., K
\end{aligned} \tag{41}$$

$$dthu_m \le thuo - tci_{m,1} + \Gamma \times (1 - zh_m) \quad m \in CU \quad (42)$$

$$dtcu_l \le thi_{l,K} - tcuo + \Gamma \times (1 - zc_l) \quad l \in HU$$
 (43)

$$dtc_{l,m,k}, dth_{l,m,k} \ge \varepsilon$$
  $(l,m) \in MA, k = 1, 2, ..., K$  (44)

Logical constraints needed to determine the existence of a heat exchanger:

$$z_{l,m,k}, zh_m, zc_l = 0, 1$$
 (45)

$$q_{l,m,k} - \Omega \times z_{l,m,k} \le 0 \quad (l,m) \in MA, k = 1, 2, ..., K$$
 (46)

$$qc_l - \Omega \times zc_l \le 0 \quad l \in HU$$
 (47)

$$qh_m - \Omega \times zh_m \le 0 \quad m \in CU$$
 (48)

Feasibility of temperatures:

$$tho_{l_1} \ge thout_{l_2} \quad l_2 \in HM$$
 (49)

$$tco_{m_2} \le tcout_{m_2} \quad m_2 \in CM \tag{50}$$

$$thi_{l,k} \ge tho_{l,k} \quad l \in HM, k = 1, 2, ..., K$$
 (51)

$$tco_{m,k} \ge tci_{m,k} \quad m \in CM, k = 1, 2, ..., K$$
 (52)

Assume that the temperature intervals are arranged in ascending order and are not overlapped.

$$tho_{l,k} \ge thi_{l,k+1}$$
  $l \in HM, k = 1, 2, ..., K$  (53)

$$tci_{m,k} \ge tco_{m,k+1} \quad m \in CM, k = 1, 2, ..., K$$
 (54)

4.2.4. Connections between WAN and HEN. Constraints include eqs 20, 21, and the following equations.

$$f_{l_1,l_2} = \sum_{k=1}^{K+1} \operatorname{trh}(l_1, l_2, k) \quad l_1 \in \operatorname{HM} \text{ or } l_2 \in \operatorname{HM}$$
 (55)

$$f_{m_1, m_2} = \sum_{k=1}^{K+1} \operatorname{trc}(m_1, m_2, k) \quad m_1 \in CM \text{ or } m_2 \in CM$$
 (56)

Energy balance at process inlet point *j*:

$$rqh_{l_{2}} = fh_{l_{2}} \times tho_{l_{2}} \times cp \quad l_{2} \in HM \cap HD$$

$$rqh_{l_{2}} = \left(\sum_{l_{1} \in HN \cap HS} (trh_{l_{1}, l_{2}, K+1} \times thin_{l_{1}})\right)$$

$$+ \sum_{l_{1} \in HM \cap HS} \sum_{k=1}^{K+1} (trh_{l_{1}, l_{2}, k} \times tho_{l_{1}, k-1}))$$

$$\times cp \quad l_{2} \in HN \cap HD$$
(59)

$$\operatorname{rqc}_{m_{2}} = \operatorname{fc}_{m_{2}} \times \operatorname{tco}_{m_{2}} \times \operatorname{cp} \quad m_{2} \in \operatorname{CM} \cap \operatorname{CD}$$

$$\operatorname{rqc}_{m_{2}} = \left( \sum_{m_{1} \in \operatorname{CN} \cap \operatorname{CS}} (\operatorname{trc}_{m_{1}, m_{2}, 1} \times \operatorname{tcin}_{m_{1}}) \right)$$

$$+ \sum_{m_{1} \in \operatorname{CM} \cap \operatorname{CS}} \sum_{k=1}^{K+1} (\operatorname{trc}_{m_{1}, m_{2}, k} \times \operatorname{tco}_{m_{1}, k}))$$

$$\times \operatorname{cp} \quad m_{2} \in \operatorname{CN} \cap \operatorname{CD}$$

$$(61)$$

Nonnegative constraint:

$$f_{l,j}$$
, trh<sub>l<sub>1</sub>,l<sub>2</sub>,k</sub>, trc<sub>m<sub>1</sub>,m<sub>2</sub>,k</sub>, fh<sub>l,k</sub>, fc<sub>m,k</sub>, q<sub>l,m,k</sub>, qh<sub>m</sub>, qc<sub>l</sub>  $\geq 0$  (62)

4.2.5. Objective Function. The total cost of WAHEN is composed of annual utility costs and capital costs. To calculate the capital cost of heat exchangers, the logarithmic mean temperature difference is approximated according to the work of Chen. <sup>29</sup> The design problem can then be formulated as the following MINLP problem:

$$\begin{split} & \min \text{CCU} \sum_{m \in \text{CU}} \text{qc}_m + \text{CHU} \sum_{l \in \text{HU}} \text{qh}_l + \text{CFW} \sum_{i \in P} f_{w,i} \\ & + \sum_{k=1}^K \sum_{(l,m) \in \text{MA}} \text{CF}_{l,m} z_{l,m,k} + \sum_{m \in \text{CU}} \text{CF}_m \text{zh}_m \\ & + \sum_{l \in \text{HU}} \text{CF}_l \text{zc}_l + \sum_{(l,m) \in \text{MA}} \sum_{k=1}^K \text{CO}_{l,m} [q_{l,m,k} / \\ & (U_{l,m} (\text{dth}_{l,m,k} \text{dtc}_{l,m,k} (\text{dth}_{l,m,k} + \text{dtc}_{l,m,k}) / 2)^{1/3})]^{B_{l,m}} \\ & + \sum_{l \in \text{HU}} \text{CO}_l [\text{qc}_l / (U_l ((\text{tho}_l - \text{tcui}) \text{dtcu}_l \\ & (\text{dtcu}_l + \text{tho}_l - \text{tcui}) / 2)^{1/3})]^{B_l} \\ & + \sum_{m \in \text{CU}} \text{CO}_m [\text{qh}_m / (U_m ((\text{thui} - \text{tco}_m) \text{dth} u_m \\ & (\text{dthu}_m + \text{thui} - \text{tco}_m) / 2)^{1/3})]^{B_m} \end{split}$$

subject to eqs 15-19, 20, 21, and 24-62.

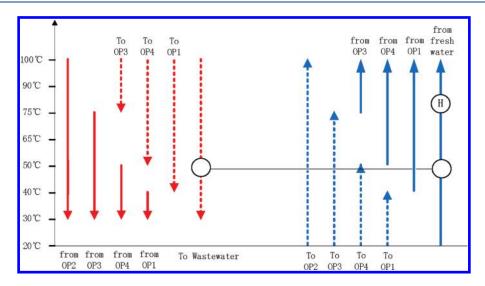


Figure 10. Match results of the MILP problem for example 1 case a.

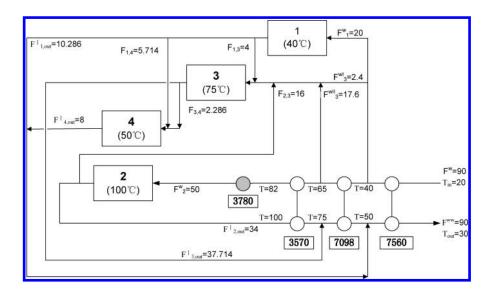


Figure 11. The HEN and WAN results for example 1 case a.

Table 3. Result Comparison of Example 1 Case a (I)

origin of method	ref 11	ref 14	ref 23	ref 24	our approach
method type	graphica	graphical	simultaneous optimization	simultaneous optimization	sequential optimization
freshwater (kg/s)	90	90	90	90	90
hot utility (KW)	4265	3780	3767	3780	3780
cold utility (KW)	485	0	0	0	0
number of heat exchangers	5	4	4	5	4

Table 4. Result Comparison of Example 1 Case a (II)

	heat exchanger area $(m^2)$	heater area (m²)	total operating cost per year (M\$)	annual HEN capital cost (M\$)	TAC (M\$)
ref 23	3498.4	132.2	7.671	0.622	8.293
our approach	3363.3	132.6	7.674	0.601	8.275

# 5. CASE STUDIES

In this section, all of the previously presented procedures are applied to the design of WAHEN for three examples. The first two examples are selected from literature in which both separate

Table 5. Cost and Operating Parameters for Example 1 Case b, Example 2 and 3

parameter		parameter		parameter	
CCU	12.6 \$/kw	CFF	50,000 \$	tcui	15 °C
CHU	136.8 \$/kw	U	$0.86~\text{kw/(m}^2~^\circ\text{C)}$	tcuo	20 °C
			$1.2 \text{ kw/(m}^2  ^{\circ}\text{C})$		
			(heater)		
CFW	1500 \$•h/t	В	0.6	thui	120 °C
CF	8600 \$	$\Delta T_{ m min}$	10 °C	thuo	120 °C
CO	1200 \$				

treating and uniform treating of wastewater are considered, while the third example is from a real PVC plant. Both the MILP and MINLP models presented are programmed in GAMS<sup>30</sup> and solved by the CPLEX solver and the DICOPT solver, respectively. Inside the DICOPT solver, CPLEX is adopted as the MIP solver while the NLP solver rotates among SNOPT, CONOPT, and MINOS between iterations. For the MINLP problem, it would clearly be desirable to start with a "good" initial guess for achieving the network structure. The solution of the MILP model provides the set of matches MA, and the heat exchanged at the intervals of each match  $q_{l,m,k}$ . On the basis of this information, an initial guess of the WAHEN superstructure can be obtained which will provide a good initial point for the numerical solution procedure.

**5.1. Example 1.** The first example is the one used in section 3. Its process data is presented in Table 1. We consider this example in two cases: case a, wastewater streams are merged and sent to

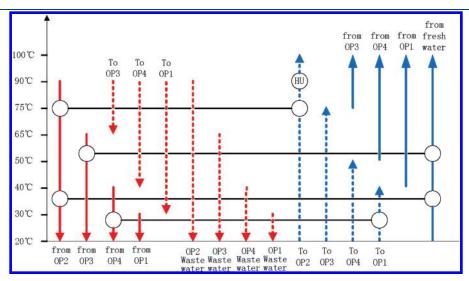


Figure 12. Targeted stream matches of example 1 case b.

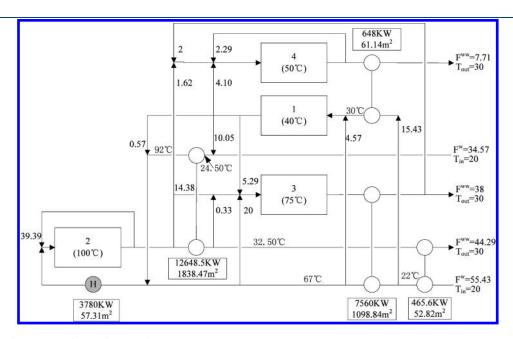


Figure 13. Network structure of example 1 case b.

treatment; case b, wastewater streams are sent to water treatment individually. Case a was also adopted by several authors, <sup>14,23,24</sup> while case b was only studied by Bagajewicz et al. <sup>18</sup> In case a, the identified hot and cold streams are shown in Figure 4. The cost and operating parameters are adopted from Bogataj and Bagajewicz<sup>23</sup> as shown in Table 2. Solving the MILP problem of the first step results in two stream matches as illustrated in Figure 10. They are a match between freshwater stream and wastewater stream and a match between freshwater stream and hot utility. Substituting these matches into the MINLP problem of the second step, the detailed WAN and HEN network structure is obtained as shown in Figure 11. From Figure 11 we can see that the minimum freshwater and hot utility consumption are 90 kg/s and 3780 KW, respectively, which are the same as those obtained by Savulscu et al., <sup>11</sup> Leewongtanawit and

Table 6. Overall Operating and Capital Costs for Example 1 Case b

costs (k\$)
517.1
135.0
273.0
925.1

Table 7. Data for Example 2<sup>a</sup>

process number	mass load of contaminant $(g/s)$	C <sub>in</sub> <sup>max</sup> (ppm)	C <sub>out</sub> <sup>max</sup> (ppm)	temperature (°C)
1	2.0	25	80	40
2	2.88	25	90	100
3	4.0	25	200	80
4	3.0	50	100	60
5	30.0	50	800	50
6	5.0	400	800	90
7	2.0	400	600	70
8	1.0	0	100	50

 $<sup>^</sup>a$  Temperature of fresh water,  $T_{\rm w}$  = 20°C; temperature of wastewater,  $T_{\rm out}$  = 30°C.

Kim, <sup>14</sup> and Dong et al. <sup>24</sup> One heater and three heat exchangers are employed to achieve the utility consumption. These numbers also agree the results of Bogataj and Bagajewicz<sup>23</sup> and Leewongtanawit and Kim. <sup>14</sup> The detailed results comparison with the other works is provided in Table 3 and Table 4. As shown in these tables, the obtained results are close. Therefore, the graphical methods, the simultaneous optimization, and the sequential optimization methods are efficient in this simple case a of example 1. However, applicabilities in examples of larger scale are seldom reported. So far, for single contaminant problems, only two examples in the literature were larger than this case. Both of the two examples were provided by Bagajewicz et al. <sup>18</sup> and solved by sequential approach. To test the applicability of the proposed approach, we will solve these two examples in the following example 1 case b and example 2.

Now, consider case b. Apart from case a, there are four wastewater streams in case b. Consequently, the number of identified hot and cold streams are 11 and 8, respectively, as shown in Figure 12. The cost factors, minimum temperature approach  $\Delta T_{\rm min}$ , and inlet/outlet utility temperatures of case b are are shown in Table 5. These parameters also hold for example 2 and 3. Applying P1 to this case b of example 1, the utility cost and the stream match targets are derived. The total cost is 902.1 k \$, with the freshwater, hot utility, and cold utility consumptions of 90 t/h, 3780 kw, and 0 kw, respectively. The resulting matches are illustrated in Figure 12, and the number of matches is five. Next, the resulting targets are used for the detailed WAN and HEN design. P2 is applied to the problem by loading the match targets of P1. The solution to the HEN results in a network containing four heat exchangers and one heater. Figure 13 shows

Table 8. Targeted Stream Matches in Case b of Example 2

match number	hot stream	cold stream
1	outlet of OP2	inlet of OP6
2	outlet of OP3	inlet of OP2
3	outlet of OP4	freshwater
4	outlet of OP5	freshwater
5	outlet of OP6	freshwater
6	hot utility	inlet of OP2

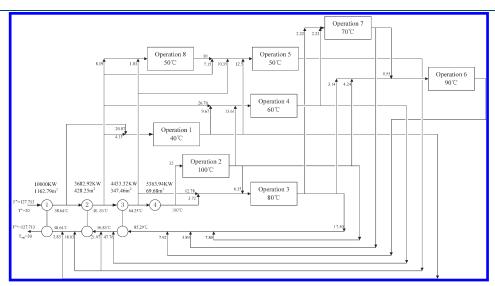


Figure 14. Network structure of example 2 case a.

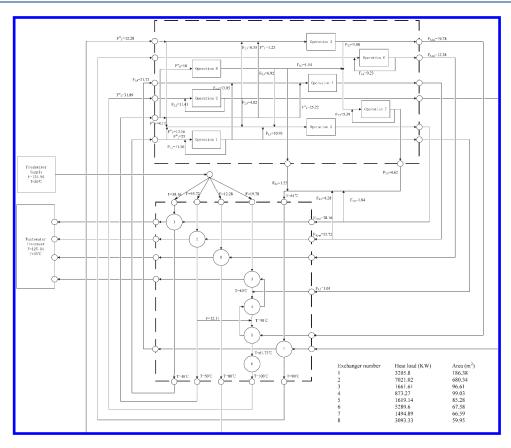


Figure 15. Network structure of example 2 case b.

Table 9. Result Comparison of Example 2

	original design (case b)	new design (case b)	new design (case a)
freshwater (kg/s)	125.94	125.94	127.713
hot utility (KW)	5290	5290	5363.94
heat exchanger area		1341.76	2008.18
heat exchanger unit	12	8	4
annual energy cost (k\$)		723.6	733.8
annual water cost (k\$)		680.1	689.6
capital cost (k\$)		279.2	218.3
total annual cost (k\$)		1682.9	1641.7

the resulting design of both WAN and HEN, while the operating and capital costs are presented in Table 6. The operating cost is the same as those reported by Bagajewicz et al., <sup>18</sup> but the number of heat exchanging units is smaller than the reported seven.

**5.2. Example 2.** The second example is a large system from Bagajewicz et al. The system consists of eight process operations and the data are illustrated in Table 7. This example is also considered in two cases: case a, uniform treating of wastewater; case b, separate treating of wastewater. For case a, a number of 16 hot and 16 cold streams can be identified from the previous definition. After applying P1 to this case, the number of targeted matches is two. One is between freshwater (CS stream) and wastewater (HD stream), and the other one is between freshwater and hot utility. In addition, the resulting utility consumptions are freshwater, 127.71 kg/s; hot utility, 5363.94

KW; and cold utility, 0 KW; and the resulting total cost is  $152.3 \, k$  \$. The final network structure provided by solving P2 is presented in Figure 14. As shown in the figure, there are four heat exchangers in the final design.

For case b, because wastewater is treated separately, the number of hot streams is increased to 23, while the number of cold streams remains unchanged. In the targeting step, the number of matches is obtained as six, and the detailed matches are shown in Table 8. In the design step, the network structure is obtained as shown in Figure 15. In the obtained network structure, there are a number of eight heat exchangers whose heat load and area parameters are also presented in the figure. Freshwater and wastewater streams are participated in the HEN. Besides, process to process streams which have been ignored by another model<sup>23</sup> are also involved in the HEN structure. The comparisons between the original design and the new designs (case a and case b) are presented in Table 9. Although we do not have the economic data of the original solution, one still can conclude from Table 9 that the solution obtained by our method is much simpler than the one reported by Bagajewicz et al. 18

**5.3. Example 3.** The third example is from a real PVC plant, and the basic flowchart is shown in Figure 16. In the plant, vinyl chloride (VC) polymerization is carried out in a polymerization reactor with deionized water environment. After the polymerization, slurry from the reactor is transferred to a stripper for removal of unreacted VC, and then is pumped to a centrifuge for separation of the polymer and water. The whole system is sensitive to ionic species, especially calcium and magnesium ions, because they can affect the performance of the reaction.

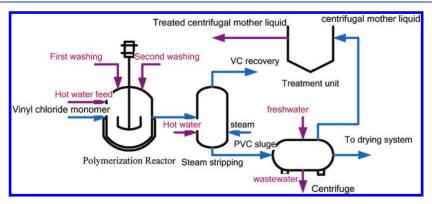


Figure 16. Flow sheet of example 3.

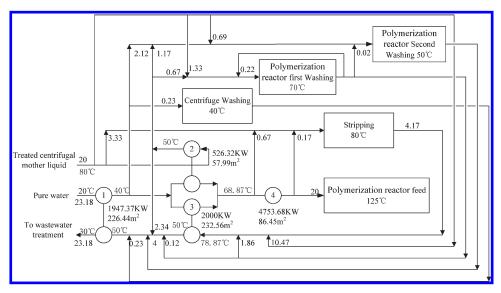


Figure 17. Network structure of example 3.

Table 10. Data for Example 3

process name	contaminant mass load $(g/s)$	C <sub>in</sub> <sup>max</sup> (ppm)	C <sub>out</sub> <sup>max</sup> (ppm)	temperature (°C)
polymerization reactor feed		0		125
polymerization reactor	1	150	600	70
first washing polymerization reactor second washing	0.6	50	200	50
stripping centrifuge washing	3 0.07	80 100	800 300	80 40

Table 11. Water Source Condition in Example 3

source item	contaminant concentration (ppm)	temperature (°C)	annual cost (k\$/t)
pure water	0	20	36
treated centrifugal mother liquid	100	80	1

Consequently, total hardness is taken as the single contaminant. Table 10 gives the mass load, contaminant, and temperature data

Table 12. Targeted Stream Matches in Example 3

match number	hot stream	cold stream
1	treated centrifugal mother liquid	pure water
2	Wastewater	pure water
3	hot utility	pure water

Table 13. Overall Operating and Capital Costs for Example 3

items	costs (k\$)
annual energy cost	650.3
annual water cost	854.5
capital cost	128.2
Total cost	1633.0

of the process units. The plant has two water sources, pure water and treated centrifugal mother liquid, whose concentration, temperature, and cost are shown in Table 11. The upper bound of treated centrifugal mother liquid supply is 20 t/h. Moreover, the wastewater discharge are treated uniformly and the environmental temperature limit is given as 30 °C in this case. As shown in Table 12, all the three targeted matches are related to pure water. The final network structure provided by solving P2 is

presented in Figure 17, while the operating and capital costs are summarized in Table 13.

# 6. CONCLUSION

The synthesis problem of heat integrated water networks has been considered. A systematic targeting and design procedure has been proposed that accounts for the splitting and nonisothermal mixing alternatives in the network. In the targeting stage, all possible hot and cold streams are implemented in the HEN for screening reasonable heat exchange matches. In the design stage, the superstructure of WAN and HEN are combined to yield an MINLP model. Solving this model, simple network structures are derived that feature the minimum total cost.

The proposed procedure features two important properties. First, a novel hot and cold stream labeling strategy has been introduced. Using the proposed approach, the number of hot and cold streams is constrained to a relative small value while maintaining the diversity of potential heat exchange matches. Second, the resulting matches of the targeting stage would help the synthesis stage capture some unique network structures that might be ignored by heuristics.

Three examples have been presented including a large scale problem and a new application to the chlor-alkali industry. The solutions involve both wastewater uniform and separate treating case. The results clearly show that the proposed method is efficient and can be used for large scale problems.

# AUTHOR INFORMATION

#### **Corresponding Author**

\*E-mail: grong@iipc.zju.edu.cn; wangjd@zju.edu.

# ACKNOWLEDGMENT

The financial support was provided by the Specialized Research Fund for the Doctoral Program of Higher Education (No: 20100101110132) and the national high technology research and development program of China (No: 2009AA044701).

# **■ NOMENCLATURE**

```
B = exponent parameter for area cost
C = contaminant concentration, ppm
CP = set of cold flow, CP = \{(i,j)|i \in \tilde{P}, j \in \tilde{P}, t_i < t_i\}
C = \text{set of cold stream}, C = \{m | m \in CS \cup CD\}
CCU = annual unit cost for cold utility ($/kw)
CD = set of cold demand stream, CD = \{m_2 | m_2^e = j, j \in CP\}
CF = fixed charge for heat exchangers ($)
CFF = cost coefficient for stream matches ($)
CFW = annual unit cost for freshwater (\$/t)
CHU = annual unit cost for hot utility (\$/kw)
CO = area cost coefficient (\$/m^2)
CS = set of cold source stream, CS = \{m_1 | m_1^s = i, i \in CP\}
CN = set of not matched cold stream, CN = \{m | m \notin MA, m \in C\}
CM = set of matched cold stream, CM = \{m | m \in MA\}
CM_l = set of cold stream that matched with hot stream l
CU = set of cold stream that matched with hot utility
cp = stream heat capacity, J \cdot kg^{-1} \cdot {}^{\circ}C^{-1}
CP = set of cold flow, CP = \{(i,j)|i \in \tilde{P}, j \in \tilde{P}, t_i < t_j\}
CT = set of cold stream transfer match, CT = \{m_1, m_2 | t_{m1}^s < t_{m2}^e\}
```

```
stream m_2, CT_{m2} = \{m_1 | (m_1, m_2) \in CT\}
dthu_m = temperature approach for the match of cold stream m
          and hot utility
dtcu_l = temperature approach for the match of hot stream l and
         cold utility
f = \text{water flow rate, kg} \cdot \text{s}^{-1}
fi_i = outlet water flow rate of process i, kg \cdot s^{-1}
f_{j_i} = inlet water flow rate of process j_i, kg·s<sup>-1</sup>
fh_l = total water flow rate of hot stream l, kg · s^{-1}
fh_{l,k} = water flow rate of hot stream l in interval k, kg \cdot s^{-1}
fc_m = total water flow rate of cold stream m, kg \cdot s
fc_{m,k} = water flow rate of cold stream m in interval k, kg \cdot s^{-1}
HP = set of hot flow, HP = \{(i,j)|i\in P, j\in P, t_i > t_j\}
H = \text{set of hot stream}, H = \{l | l \text{ HS} \cup \text{HD}\}
HD = set of hot demand stream, HD = \{l_2 | l_2^e = j, j \in HP\}
HS = set of hot source stream, HS = \{l_1|l_1^s = i, i \in HP\}
HT = set of hot stream transfer match, HT = \{(l_1, l_2) | t_{l1s} > t_{l2e}\}
HT_{l1} = set of hot demand streams that receive flow from hot
         source stream l_1, HT_{l1} = \{l_2 | (l_1, l_2) \in HT\}
HT_{12} = set of hot source streams that flow to hot demand stream
         l_2, HT_{l2} = \{l_1 | (l_1, l_2) \in HT\}
HN = set of not matched hot stream, HN = \{l | l \notin MA, l \in H\}
HM = set of matched hot stream, <math>HM = \{l | l \in MA\}
HM_m = set of hot stream that matched with cold stream m
HU = set of hot stream that matched with cold utility
K = \text{total number of intervals}
L = \text{mass load of water using process, g} \cdot \text{s}^{-1}
MA = set of permitted match, MA = \{(l,m)|l \in H, m \in C, \text{ match}\}
       between l and m is permitted}
P = \text{set of water using process}
\hat{P} = set of water source point, = \{P, w\}
\tilde{P} = set of water sink point, = \{P_i w w_i\}
qc_l = heat exchanged between hot stream l and cold utility, KW
qh_m = heat exchanged between cold stream m and hot utility, KW
q_{l,m,k} = heat exchanged between hot stream l and cold stream m in
        interval k, KW
rqh_l = residual energy of hot demand stream l leaving HEN
rqc_m = residual energy of cold demand stream m leaving HEN
         operator
t = \text{water temperature, } ^{\circ}\text{C}
\Delta T_{\min} = minimum temperature approach, °C
tci_{m,k} = inlet temperature of cold stream m at interval k, ^{\circ}C
tco_{m,k} = outlet temperature of cold stream m at interval k, ^{\circ}C
tcin = initial temperature of cold source stream, °C
tcout = upper bound of outlet temperature of cold matched
          stream, °C
tcui = inlet temperature of cold utility, °C
tcuo = outlet temperature of cold utility, °C
thi<sub>l,k</sub> = inlet temperature of hot stream l at interval k, ^{\circ}C
tho<sub>lk</sub> = outlet temperature of hot stream l at interval k, {}^{\circ}C
thin = initial temperature of hot source stream, °C
thout = lower bound of outlet temperature of hot matched
          stream, °C
thui = inlet temperature of hot utility, °C
thuo = outlet temperature of hot utility, °C
to_k = outlet temperature of temperature interval k
trc_{m1,m2,k} = flow rate transferred from coldstream m_1 to m_2 in
             interval k, °C
```

 $CT_{m1}$  = set of cold demand streams that receive flow from cold

source stream  $m_1$ ,  $CT_{m1} = \{m_2 | (m_1, m_2) \in CT\}$  $CT_{m2}$  = set of cold source streams that flow to cold demand  $\operatorname{trh}_{l1,l2,k} = \operatorname{flow}$  rate transferred from hot stream  $l_1$  to  $l_2$  in interval k.  $^{\circ}\mathrm{C}$ 

U = overall heat transfer coefficient

w = fresh water

ww = Wastewater

 $z_{l,m,k}$  = binary variable to denote the existence of match (l,m) in interval k

 ${\rm zh}_m={\rm binary}$  variable to denote that hot utility exchanges heat with cold stream m

 $zc_l$  = binary variable to denote that cold utility exchanges heat with hot stream l

 $zsd_{l,m}$  = binary variable to denote the existence of match (l,m)

 $\Omega$  = an upper bound for heat exchange, KW

 $\Gamma$  = an upper bound for temperature difference, °C

#### Superscript

max = maximum

#### Subscript

in = at the inlet of a process

k = index for interval 1, ..., K and temperature location 1, ..., K + 1

i =outlet of process

j = inlet of process

l = hot stream

 $l_1$  = hot source stream

 $l_2$  = hot demand stream

m = cold stream

 $m_1$  = cold source stream

 $m_2$  = cold demand stream

out = at the outlet of a process

#### ■ REFERENCES

- (1) Bagajewicz, M. A review of recent design procedures for water networks in refineries and process plants. *Comput. Chem. Eng.* **2000**, 24 (9-10), 2093-2113.
- (2) Foo, D. C. Y. State-of-the-art review of pinch analysis techniques for water network synthesis. *Ind. Eng. Chem. Res.* **2009**, 48 (11), 5125–5159.
- (3) Jezowski, J. Review of water network design methods with literature annotations. *Ind. Eng. Chem. Res.* **2010**, 49 (10), 4475–4516.
- (4) Linnhoff, B. Pinch analysis—a state-of-the-art overview. Chem. Eng. Res. Des. 1993, 71 (A5), 503–522.
- (5) Furman, K. C.; Sahinidis, N. V. A critical review and annotated bibliography for heat exchanger network synthesis in the 20th century. *Ind. Eng. Chem. Res.* **2002**, *41* (10), 2335–2370.
- (6) Savulescu, L. E.; Alva-Argaez, A. Direct heat transfer considerations for improving energy efficiency in pulp and paper Kraft mills. *Energy* **2008**, 33 (10), 1562–1571.
- (7) Manan, Z. A.; Tea, S. Y.; Alwi, S. R. W. A new technique for simultaneous water and energy minimisation in process plant. *Chem. Eng. Res. Des.* **2009**, 87 (11), 1509–1519.
- (8) Kim, J.; Kim, J.; Kim, J.; Yoo, C.; Moon, I. A simultaneous optimization approach for the design of wastewater and heat exchange networks based on cost estimation. *J. Clean. Prod.* **2009**, *17* (2), 162–171.
- (9) Savulescu, L.; Smith, R. Simultaneous Energy and Water Minimisation. AIChE Annual Meeting, Miami, FL, 1998.
- (10) Savulescu, L.; Kim, J.; Smith, R. Studies on simultaneous energy and water minimisation—Part I: Systems with no water re-use. *Chem. Eng. Sci.* **2005**, *60* (12), 3279–3290.
- (11) Savulescu, L.; Kim, J.; Smith, R. Studies on simultaneous energy and water minimisation—Part II: Systems with maximum re-use of water. *Chem. Eng. Sci.* **2005**, *60* (12), 3291–3308.

- (12) Savulescu, L.; Sorin, M.; Smith, R. Direct and indirect heat transfer in water network systems. *Appl. Therm. Eng.* **2002**, 22 (8), 981–988.
- (13) Sorin, M.; Savulescu, L. On minimization of the number of heat exchangers in water networks. *Heat Transfer Eng.* **2004**, *25* (5), 30–38.
- (14) Leewongtanawit, B.; Kim, J.-K. Improving energy recovery for water minimisation. *Energy* **2009**, 34 (7), 880–893.
- (15) Sahu, G. C.; Bandyopadhyay, S. Energy conservation in water allocation networks with negligible contaminant effects. *Chem. Eng. Sci.* **2010**, *65* (14), 4182–4193.
- (16) Feng, X.; Li, Y.; Yu, X. Improving energy performance of water allocation networks through appropriate stream merging. *Chin. J. Chem. Eng.* **2008**, *16* (3), 480–484.
- (17) Feng, X.; Li, Y.; Shen, R. A new approach to design energy efficient water allocation networks. *Appl. Therm. Eng.* **2009**, 29 (11–12), 2302–2307.
- (18) Bagajewicz, M.; Rodera, H.; Savelski, M. Energy efficient water utilization systems in process plants. *Comput. Chem. Eng.* **2002**, *26* (1), 59–79
- (19) Liao, Z. W.; Yang, Y. R.; Wang, J. D.; Jiang, B. B. Optimization of energy efficient water utilization systems. *J. Chem. Ind. Eng., Chin.* **2007**, 58 (2), 396–402.
- (20) Liao, Z. W.; Wu, J. T.; Jiang, B. B.; Wang, J. D.; Yang, Y. R. Design energy efficient water utilization systems allowing operation split. *Chin. J. Chem. Eng.* **2008**, *16* (1), 16–20.
- (21) Leewongtanawit, B.; Kim, J.-K. Synthesis and optimization of heat-integrated multiple-contaminant water systems. *Chem. Eng. Process.: Process Intensification* **2008**, 47 (4), 670–694.
- (22) Floudas, C. A.; Ciric, A. R. Strategies for overcoming uncertainties in heat exchanger network synthesis. *Comput. Chem. Eng.* **1989**, 13 (10), 1133–1152.
- (23) Bogataj, M.; Bagajewicz, M. J. Synthesis of non-isothermal heat integrated water networks in chemical processes. *Comput. Chem. Eng.* **2008**, 32 (12), 3130–3142.
- (24) Dong, H.-G.; Lin, C.-Y.; Chang, C.-T. Simultaneous optimization approach for integrated water-allocation and heat-exchange networks. *Chem. Eng. Sci.* **2008**, *63* (14), 3664–3678.
- (25) Dong, H.-G.; Lin, C.-Y.; Chang, C.-T. Simultaneous optimization strategy for synthesizing heat exchanger networks with multi-stream mixers. *Chem. Eng. Res. Des.* **2008**, 86 (3), 299–309.
- (26) Savelski, M.; Bagajewicz, M. On the optimality conditions of water utilization systems in process plants with single contaminants. *Chem. Eng. Sci.* **2000**, *55* (21), 5035–5048.
- (27) Papoulias, S.; Grossmann, I. A structural optimization approach in process synthesis—II: Heat recovery networks. *Comput. Chem. Eng.* **1983**, 7 (6), 707–721.
- (28) Yee, T. F.; Grossmann, I. E. Simultaneous optimization model for heat integration—II: Heat exchanger network synthesis. *Comput. Chem. Eng.* 1990, 14 (10), 1165–1184.
- (29) Chen, J. J. J., Letter to the editors: Comments on improvement on a replacement for the logarithmic mean. *Chem. Eng. Sci.* **1987**, 42, 2488-2489.
- (30) Brooke, A.; Kendrick, D.; Meeraus, A.; Raman, R., GAMS. a User's Guide. GAMS Development Corporation: Washington, DC, 1998.