Simultaneous Integration of Water and Energy in Heat-Integrated Water Allocation Networks

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This article proposes a new methodology for simultaneous integration of water and energy in heat-integrated water allocation networks (WAHEN). A novel disjunctive model is first developed to determine an optimal water allocation network (WAN) where water and energy are integrated in one step. Based on the optimal WAN, a detailed heat exchanger network (HEN) to satisfy the utility target is then synthesized. Although the final network structure is obtained through two steps, the targets of freshwater and utility are optimized simultaneously. The proposed method has specific advantages. First of all, it can capture a tradeoff among freshwater usage, utility consumption, and direct heat transfer by nonisothermal mixing. Second, it can greatly reduce the complexity of subsequent HEN design. Finally, it is effective for simultaneous water and energy integration in large-scale WAHEN systems. The advantages and applicability of this new method are illustrated by three examples from literature. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 2202–2214, 2015

Keywords: water allocation network, heat exchanger network, simultaneous optimization, water and energy integration, nonisothermal mixing

Introduction

Water and energy are essential resources for process industries such as refineries, food production, chemical plants, etc. Recently, due to the rapid depletion of energy resources, scarcity of freshwater and stricter environmental regulations, process industries are driven to minimize the consumption of water and energy. In a chemical process, water is usually used as a carrier of both mass and energy. Not only must water have certain quality standards but also it has to be heated up or cooled down to meet the temperatures of different operations. Therefore, strong interaction exists between water and energy utilization. Generally, the reduction of freshwater can lead to the reduction of energy consumption and vice versa.[1] The coupling of these two processes underlines the importance of performing simultaneous minimization of water and energy in heat-integrated water allocation networks (WAHEN).

The importance of simultaneous minimization of water and energy in WAHEN was first addressed by Savelski and Bagajewicz.[2] From then on, different methods, rooted in conceptual design coupled with pinch analysis or mathematical programming based on superstructures have been developed to achieve such goals. Savulescu et al.[3,4] proposed a conceptual design method for simultaneous water and energy minimization. They introduced a graphic representation, called the two-dimensional grid diagram to determine a water allocation network (WAN) with minimum water and energy consumption. Then they adopted a separate system to synthesize the heat exchanger network (HEN), considering both direct and indirect heat transfer.[5,6] Leewongtanawit and Kim[7] developed a water-energy balance diagram for WAHEN design. They applied this method to systematically investigate the influences of stream merging and splitting as well as nonisothermal mixing, to identify energy-efficient and cost-effective configurations for heat recovery and finally to synthesize single-contaminant water systems. Subsequently, Martinez-Patino et al.[8] studied the interactions between water and energy systems, and proposed a heuristic procedure—temperature vs. concentration diagram to reduce freshwater and utility consumption. Sahu and Bandyopadhyay[9] developed an energy recovery algorithm to target the minimum utility consumption before the detailed designs of WAN and HEN, but this algorithm only applied to negligible contaminant water systems. Recently, Feng et al.[10,11] and Luo et al.[12,13] studied the effects of nonisothermal mixing on the energy performance of WAN, and proposed some qualitative rules on how to avoid or eliminate energy penalty. Additionally, Hou et al.[14] explored the concepts of concentration potential and introduced a visualization tool—temperature and concentration composite curves for water and energy integration. Conceptual design methods are

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straightforward and offer the designers insights as well as controllability during the whole design process, however, they are not mathematically rigorous, and therefore, cannot guarantee the optimal energy integration of the water systems.

Mathematical programming methods have been proposed to overcome the limitation of conceptual design methods. Sequential and simultaneous approaches are two major methodologies. Bagajewicz et al.[15] developed two sequential linear programming (LP) models to minimize water usage and energy requirement, and then applied a mixed-integer linear programming model to obtain the detailed HEN. George et al.[16] and Sahu et al.[17] proposed two different kinds of sequential formulations for heat integration in fixed flow rate water allocation problems. They studied both isothermal and nonisothermal mixings of streams and proposed some theorems. Note that the above approaches rely on sequential optimization strategy, namely, first minimizing the freshwater usage and then determining the hot and cold utilities under the targeted freshwater usage. In other words, the integration of water and energy is not accomplished in one step, but two. This ignores the interaction between water usage and energy consumption, and therefore cannot guarantee the optimal conditions. For the simultaneous optimization for water and energy integration, Boix et al.[18] and Yang and Grossmann[19] developed two linear formulations to minimize freshwater and energy consumption of multicontaminant systems. Ahmetovic and Kravanja[20] combined WAN and HEN together to form a superstructure that incorporates not only direct and indirect heat transfer but also the splitting and mixing of freshwater and wastewater streams. As for the nonisothermal mixings of streams, Ahmetovic and Kravanja[21] proposed two strategies for nonisothermal mixings of process-to-process streams and applied them to improve the network designs. Bogataj and Bagajewiz[22] and Liao et al.[23] modified a stage-wise superstructure to deal with the mixing and splitting of streams in HEN and formulated a mixed-integer nonlinear programming (MINLP) problem for the network design. In addition, Dong et al.[24] adopted a modified state-space representation to incorporate water reuse and treatment as well as direct and indirect heat transfer, and formulated an MINLP problem for simultaneous synthesis of WAN and HEN. They introduced a stochastic perturbation procedure to generate reliable initial guesses and developed an interactive iteration method to guide the search toward optimal conditions. Besides of water and energy integration, Jimenez-Gutierrez et al.[25] considered properties integration and presented an MINLP formulation for simultaneous mass, energy, and properties integration. Although these contributions realized simultaneous integration of water and energy, their models are very complicated and hardly applied to large-scale WAHEN systems. Therefore, it is of necessity to establish a new mathematical model to address this research gap. The main focus of the present article is the development of such a model.

In this article, we propose a new method for WAHEN synthesis, whose design procedure is shown in Figure 1. A disjunctive model is first developed to determine an optimal WAN using simultaneous integration of water and energy. Based on the optimal WAN, a detailed HEN to satisfy the utility target is then synthesized. The proposed method makes full use of nonisothermal mixing of streams and achieves simultaneous minimization of freshwater and utility consumption. Furthermore, it is applicable to large-scale problems. Therefore, the proposed method presents a reasonable and effective strategy for WAHEN synthesis. The remainder of the article is organized as follows. A problem statement is first presented and a brief introduction of Generalized Disjunctive Programming (GDP) is then given. The mathematical formulation for simultaneous integration of water and energy is derived next. In the following section, three examples are presented to demonstrate the effectivity and applicability of the proposed method. Finally, conclusions about this work are drawn.

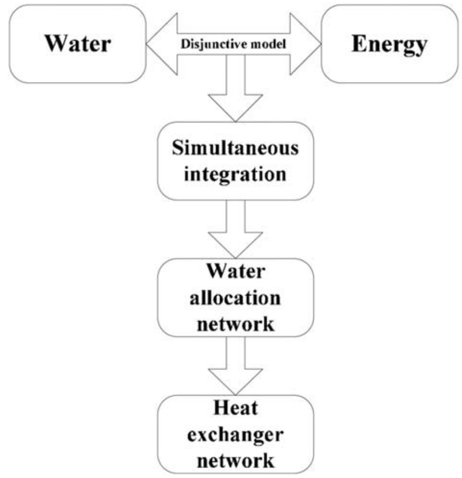

Figure 1. The design procedure of WAHEN synthesis.

Problem Statement

The problem addressed in this article can be stated as follows:

Given is set of water-using units P that require water of a certain quality and temperature. The objective is to derive an optimal WAN using simultaneous integration of water and energy and determine a HEN between hot and cold streams that satisfies the targeted utility consumption. To simplify the synthesis problem and facilitate the formulation of mathematical model for the simultaneous water and energy integration, the following assumptions are adopted:

1. The data (including maximum inlet and outlet concentration of contaminant, operating temperature, and contaminant mass load) for each water-using unit are specified and constant,
2. Water-using units operate isothermally and continuously, and no water and heat losses or gains are considered;
3. Freshwater is free of contaminant, and no concentration constraints are set for wastewater,
4. All water streams have constant heat capacity ($cp = 4.2$ kJ kg^{-1} K^{-1}).

Assumption (2) is general and usually adopted in WAHEN synthesis[9–11,22–24] for the purpose of simplification. In fact, if water and heat losses or gains are considered, the model proposed in the following section shall be still applicable as long as mass and energy balance equations for water and heat losses or gains are added into the model. In that case, the losses or gains must be specified. Generally, the heat capacity of water depends on the temperature. However, assumption (4) is usually adopted as the heat capacity shift caused by temperature change would give no effect on the results of HEN synthesis. In such a condition, assumption

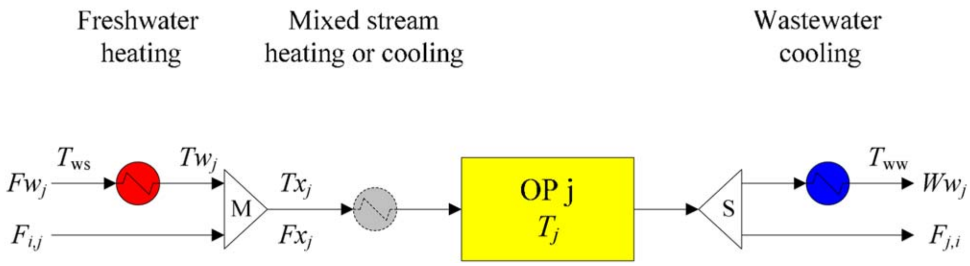

Figure 2. Superstructure of water allocation network including heat transfer.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

(4) would add no effect on the accuracy of the formulation if the concentration of the contamination in the water is low enough so that the change in the heat capacity of the contaminated water is negligible. This is the case for the problem addressed in the present article because contaminant concentrations in water streams are in the order of ppm.

Generalized Disjunctive Programming

GDP is a form to model discrete/continuous optimization problems by using algebraic equations, disjunctions, and logic propositions. Comprehensive review of GDP can be found in Grossmann and Trespalacios.[26] For the problem of simultaneous water and energy integration in WAHEN, the structure of GDP has the following form

$$\begin{aligned} & \min z = f(\boldsymbol{x}) \\ s.t. \quad & g(\boldsymbol{x}) \le 0 \\ & \vee_{i \in D_k} \begin{bmatrix} Y_{ki} \\ h_{ki}(\boldsymbol{x}) \le 0 \end{bmatrix} \quad k \in K \\ & \Omega(\boldsymbol{Y}) = \text{True} \\ & \boldsymbol{x} \ge 0, Y_{ki} \in \{\text{True}, \text{False}\}, i \in D_k, k \in K \end{aligned} \tag{GDP}$$

The objective is a function of the continuous variables $\boldsymbol{x}$, representing the annual operational cost of WAHEN. The global constraints $g(\boldsymbol{x}) \le 0$ hold true regardless of the Boolean variables Y_{ki} and represent the mass balance equations of WAN. Y_{ki} only takes the value of True or False, and determines if a given term ($h_{ki}(\boldsymbol{x}) \le 0$) in a disjunction is enforced ($Y_{ki} = \text{True}$) or ignored ($Y_{ki} = \text{False}$). The disjunctions represent the heat integration equations of HEN. $\Omega(\boldsymbol{Y}) = \text{True}$ represents the set of logic propositions that relates the Boolean variables.

The GDP problem can be reformulated as MINLP problem by replacing Boolean variables Y_{ki} with binary variables y_{ki} and using Big-M formulation. The logic propositions $\Omega(\boldsymbol{Y}) = \text{True}$ can be converted into linear inequalities. The reformulated MINLP problem can be written as

$$\begin{aligned} & \min z = f(\boldsymbol{x}) \\ s.t. \quad & g(\boldsymbol{x}) \le 0 \\ & h_{ki}(\boldsymbol{x}) \le M_{ki}(1 - y_{ki}) \quad i \in D_k, k \in K \\ & \sum_{i \in D_k} y_{ki} = 1 \quad k \in K \\ & \boldsymbol{A}\boldsymbol{y} \le a \\ & \boldsymbol{x} \ge 0, y_{ki} \in \{0, 1\}, i \in D_k, k \in K \end{aligned} \tag{MINLP}$$

In this MINLP problem, the inequality constraints $h_{ki}(\boldsymbol{x}) \le M_{ki}(1 - y_{ki})$, ($i \in D_k$, $k \in K$) are the Big-M formulation of disjunctions in GDP. In this formulation, M_{ki} are the so-called Big-M parameters, which should be set to a value arbitrarily big enough so that the inequalities become redundant when $y_{ki} = 0$ ($Y_{ki} = \text{False}$) and become $h_{ki}(\boldsymbol{x}) \le 0$ when $y_{ki} = 1$ ($Y_{ki} = \text{True}$). The inequalities $\boldsymbol{A}\boldsymbol{y} \le a$ can be systematically derived from $\Omega(\boldsymbol{Y}) = \text{True}$ by using Boolean algebra rules. The MINLP problem can be solved by the existing commercial MINLP solvers. Therefore, the key part of WAHEN synthesis is the development of a GDP model for simultaneous water and energy integration, which would be described in detail in the following section.

Mathematical Formulation for Simultaneous Water and Energy Integration

A novel GDP model is developed in this section to realize simultaneous integration of water and energy in WAHEN. The GDP model is based on WAN model and LP transshipment model of HEN, and consists of mass balance equations for water and contaminant and heat integration equations with the minimum annual operational cost of WAHEN as the objective function.

Water allocation network model

A general WAN superstructure including heat transfer is shown in Figure 2. Freshwater Fw_j is heated from freshwater source temperature T_{ws} to an appropriate temperature Tw_j and then mixed with the reused water $F_{i,j}$. A mixed stream Fx_j (stream that connects mixer and water-using unit is defined as mixed stream in this article) with a start temperature Tx_j is generated. Note that mixed stream Fx_j could be either hot or cold, depending on the relationship between its start temperature Tx_j and the operating temperature T_j of water-using unit j. If mixed stream Fx_j is a cold stream, it must be heated to satisfy the operating temperature T_j. Otherwise, it must be cooled to meet T_j. The water stream from water-using unit j can be reused by water-using unit i ($F_{j,i}$) or is cooled to the temperature of wastewater T_{ww} and then discharged (Ww_j).

A linearized formulation from Savelski and Bagajewicz[27] is adopted for WAN and presented as follows:

Flow rate balance of each mixer

$$Fw_j + \sum_{i \ne j} F_{i,j} = Fx_j \quad \forall i, \ \forall j \in P \tag{1}$$

Flow rate balance of each water-using unit

$$Fw_j + \sum_{i \ne j} F_{i,j} = \sum_{i \ne j} F_{j,i} + Ww_j \quad \forall i, \ \forall j \in P \tag{2}$$

Maximum inlet concentration constraint

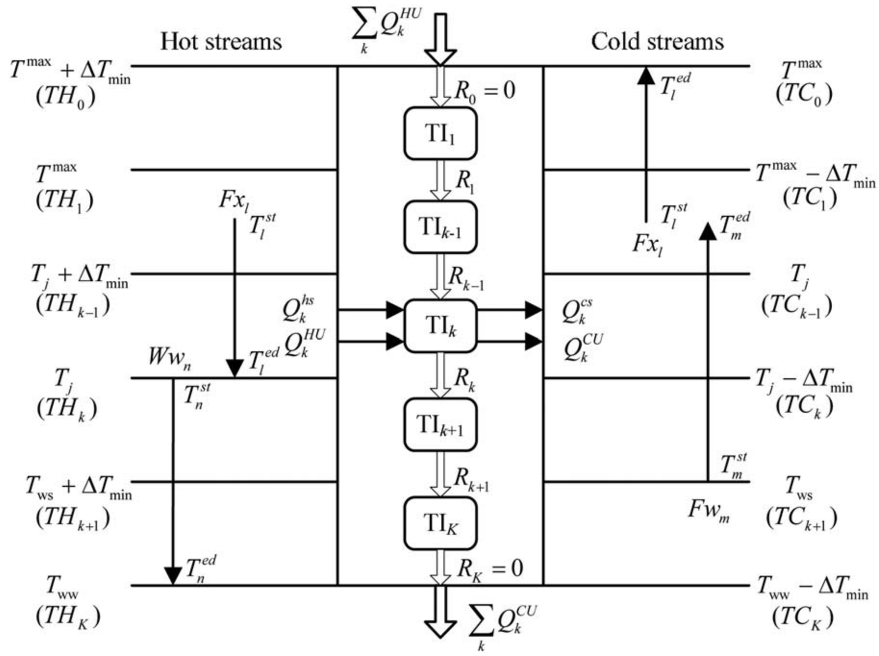

Figure 3. Extended LP transshipment model.

$$\sum_{i \neq j} F_{i,j} C_{i,\text{out}}^{\max} - Fx_j C_{j,\text{in}}^{\max} \leq 0 \quad \forall i, \ \forall j \in P \tag{3}$$

Contaminant mass balance of each water-using unit

$$\sum_{i \neq j} F_{i,j} C_{i,\text{out}}^{\max} + L_j = \left(\sum_{i \neq j} F_{j,i} + Fw_j\right) C_{j,\text{out}}^{\max} \quad \forall i, \ \forall j \in P \tag{4}$$

In order to evaluate the direct heat transfer by nonisothermal mixing in mixers, we add the following two constraints.

Energy balance of each mixer

$$Fw_j Tw_j + \sum_{i \neq j} F_{i,j} T_i = Fx_j Tx_j \quad \forall i, \ \forall j \in P \tag{5}$$

Energy balance of each mixed stream

$$cpFx_j Tx_j + Qp_j - Qn_j = cpFx_j T_j \quad \forall j \in P \tag{6}$$

It may be noted from Eq. 6 that positive variables, Qp_j and Qn_j, indicate the energy demand of mixed stream Fx_j. If $Qp_j > 0$, mixed stream Fx_j needs additional heating and is a cold stream; if $Qn_j > 0$, mixed stream Fx_j needs to be cooled and is a hot stream. Specifically, if $Qp_j = Qn_j = 0$, mixed stream Fx_j could be excluded from the subsequent HEN design since its energy demand is satisfied by the direct heat transfer in mixer. Besides, the minimization of Qp_j and Qn_j tends to maximize the direct heat transfer by nonisothermal mixing in mixer to meet the energy demand of mixed stream Fx_j.

LP transshipment model of HEN

When minimizing the external hot and cold utilities, we only consider mixed streams (MS), freshwater streams (FWS), and wastewater streams (WWS), denoted by subscript l, m, and n, respectively. This is reasonable because the energy demand of reused water streams ($F_{i,j}$) in Figure 2 is transferred to mixed streams through nonisothermal mixing. Thus, the energy demand of mixed streams, freshwater streams and wastewater streams indicates the hot and cold utilities consumed by WAN. Moreover, this keeps the model dimensionality to a manageable size because the total number of streams for utility targeting would not exceed $3N$ (N is the number of water-using units). The start and end temperatures, denoted by superscript st and ed, respectively, of mixed streams, freshwater streams, and wastewater streams in WAN superstructure and LP transshipment model are related through the following equations

$$\left.\begin{aligned} T_l^{\text{st}} &= Tx_j \\ T_l^{\text{ed}} &= T_j \end{aligned}\right\} \quad \forall l \in \text{MS}, \ \forall j \in P \tag{7}$$

$$\left.\begin{aligned} T_m^{\text{st}} &= T_{\text{ws}} \\ T_m^{\text{ed}} &= Tw_j \end{aligned}\right\} \quad \forall m \in \text{FWS}, \ \forall j \in P \tag{8}$$

$$\left.\begin{aligned} T_n^{\text{st}} &= T_j \\ T_n^{\text{ed}} &= T_{\text{ww}} \end{aligned}\right\} \quad \forall n \in \text{WWS}, \ \forall j \in P \tag{9}$$

Note that in Eqs. 7–9 only T_l^{st} (Tx_j) and T_m^{ed} (Tw_j) are variables; the others are constants. We extend the LP transshipment model of HEN[28] to optimize T_l^{st} and T_m^{ed} and determine the minimum external hot and cold utilities. Also note that mixed stream Fx_l could be either hot or cold in LP transshipment model, depending on the relationship between T_l^{st} and T_l^{ed}. The extension of the transshipment model is presented in Figure 3.

Partition of temperature intervals

Prior to using the transshipment model, the entire temperature range of mixed streams, freshwater streams, and wastewater streams should be partitioned into temperature intervals. To ensure the minimum approach temperature ($\Delta T_{\min}$) between hot and cold streams, cold temperature boundaries can be obtained by subtracting $\Delta T_{\min}$ from the corresponding hot temperature boundaries. Then, we partition the entire temperature range into temperature intervals using T_j, T_{ws}, and T_{ww} (see Figure 3, where $T^{\max} = \max\{T_j\}$). Hot and cold temperature boundaries are

Table 1. Data for Example 1

Process Number	Mass Load of Contaminant (g s^{-1})	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	2	0	100	40
2	5	50	100	100
3	30	50	800	75
4	4	400	800	50

Temperature of freshwater source T_{ws}=20°C.
Temperature of wastewater T_{ww}=30°C.

also denoted by TH and TC, respectively. From Eqs. 7–9 and Figure 3, we could know that the end temperature of mixed stream (T_l^{ed}), the start temperature of freshwater stream (T_m^{st}) and the start and end temperatures of wastewater stream (T_n^{st}, T_n^{ed}) are all on the temperature boundaries. Therefore, the relative position of mixed stream to each temperature interval depends on its start temperature (T_l^{st}) while the relative position of freshwater stream to each temperature interval depends on its end temperature (T_m^{ed}). In addition, the relative position of wastewater stream to each temperature interval is determined.

Now, let us take an example from Savulescu et al.[4] to illustrate the partition of temperature intervals. This example consists of four water-using units whose data are listed in Table 1. The partition of temperature intervals of Example 1 is shown in Figure 4.

From Figure 4, we could know:

1. For wastewater stream, the start and end temperatures (T_n^{st}, T_n^{ed}) are all on hot temperature boundaries. Therefore, the position of wastewater stream to each temperature interval is known.
2. The mixed stream that feeds to water-using unit (OP 2) with the maximum operating temperature T^{max} cannot be a hot stream. Moreover, the end temperature (T_l^{ed}) of mixed stream is on temperature boundaries.
   a. If mixed stream is a hot stream, its start temperature (T_l^{st}) may appear in the temperature intervals above T_l^{ed} but below T^{max}. To screen out these temperature intervals for hot mixed streams, we define set *HM*:

$$\text{HM}=\{(l,k)|\text{TH}_k \geq T_l^{ed} \text{ and } \text{TH}_k < T^{max}\}$$

   b. If mixed stream is a cold stream, its start temperature (T_l^{st}) may appear in the temperature intervals below T_l^{ed} but above T_{ws}. To screen out these temperature intervals for cold mixed streams, set *CM* is defined:

$$\text{CM}=\{(l,k)|TC_k < T_l^{ed} \text{ and } TC_k \geq T_{ws}\}$$

3. The start temperature of freshwater stream (T_m^{st}) is on cold temperature boundary. Its end temperature (T_m^{ed}) may appear in the temperature intervals above T_m^{st} but below T_j. we denote T_j by T_m^{up} here. Set *WM* is defined to screen out these temperature intervals for freshwater streams

$$\text{WM}=\{(m,k)|TC_k < T_m^{up} \text{ and } TC_k \geq T_{ws}\}$$

In a word, sets (HM, CM, and WM) screen out the promising temperature intervals where mixed streams and freshwater streams may be located while omitting the redundant ones, and therefore help reduce computational burden.

Heat transfer within each temperature interval

After screening out the promising temperature intervals for mixed streams and freshwater streams, we need to determine their relative positions to each promising temperature interval to compute heat transfer. For clear clarification, we characterize each temperature interval by two upper and two lower temperatures, as shown in Figure 5. The upper and lower temperatures of each temperature interval can be obtained by Eq. 10

$$\begin{aligned} &\text{TH}_k^{up}=\text{TH}_{k-1}, \quad \text{TH}_k^{lo}=\text{TH}_k \\ &\text{TC}_k^{up}=\text{TC}_{k-1}, \quad \text{TC}_k^{lo}=\text{TC}_k \qquad k=1,2,...,K \end{aligned} \tag{10}$$

The relative positions of mixed stream and freshwater stream to each temperature interval is illustrated in Figure 5. For a given temperature interval k, the start temperature of mixed stream (T_l^{st}) and the end temperature of freshwater stream (T_m^{ed}) may be located above, inside or below the temperature interval:

1. If mixed stream is a hot stream, heat exchange occurs when T_l^{st} is located above or inside temperature interval k (cases hx_1 and hx_2 in Figure 5). Otherwise hot mixed stream does not exchange heat in temperature interval k (case hx_3 in Figure 5).
2. If mixed stream is a cold stream, heat exchange occurs when T_l^{st} is located inside or below temperature interval k (cases cx_2 and cx_3 in Figure 5). Otherwise cold mixed stream does not exchange heat in temperature interval k (case cx_1 in Figure 5).
3. Freshwater stream exchanges heat when T_m^{ed} is located above or inside temperature interval k (cases ws_1 and ws_2 in Figure 5). Otherwise heat exchange does not occur (case ws_3 in Figure 5).

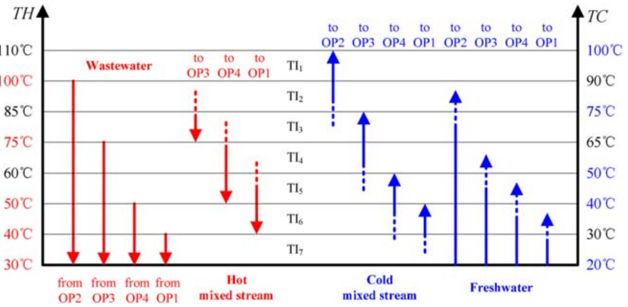

Figure 4. Partition of temperature intervals of Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

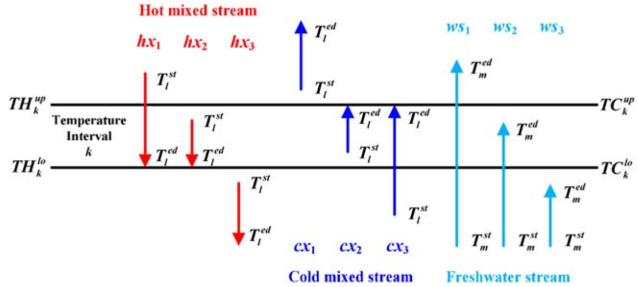

Figure 5. Relative positions of streams to temperature interval *k*.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

To model these alternatives, we define the following Boolean variables, as shown in Table 2. Three disjunctions (11–13) for hot mixed stream, cold mixed stream, and freshwater stream can be written based on the definition of Boolean variables

$$\begin{bmatrix} Y_l^{\mathrm{hx}} \\ T_l^{\mathrm{st}} > T_l^{\mathrm{ed}} \\ \begin{bmatrix} Y_{l,k}^{\mathrm{hx}_1} \\ Q_{l,k}^{\mathrm{hx}} = cpFx_l(\mathrm{TH}_k^{\mathrm{up}} - \mathrm{TH}_k^{\mathrm{lo}}) \\ T_l^{\mathrm{st}} \geq \mathrm{TH}_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{l,k}^{\mathrm{hx}_2} \\ Q_{l,k}^{\mathrm{hx}} = cpFx_l(T_l^{\mathrm{st}} - \mathrm{TH}_k^{\mathrm{lo}}) \\ \mathrm{TH}_k^{\mathrm{lo}} \leq T_l^{\mathrm{st}} \leq \mathrm{TH}_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{l,k}^{\mathrm{hx}_3} \\ Q_{l,k}^{\mathrm{hx}} = 0 \\ T_l^{\mathrm{st}} \leq \mathrm{TH}_k^{\mathrm{lo}} \end{bmatrix} \end{bmatrix} \quad \forall l,\ \forall k \in \mathrm{HM} \tag{11}$$

$$\begin{bmatrix} Y_l^{\mathrm{cx}} \\ T_l^{\mathrm{st}} \leq T_l^{\mathrm{ed}} \\ \begin{bmatrix} Y_{l,k}^{\mathrm{cx}_1} \\ Q_{l,k}^{\mathrm{cx}} = 0 \\ T_l^{\mathrm{st}} \geq TC_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{l,k}^{\mathrm{cx}_2} \\ Q_{j,k}^{\mathrm{cx}} = cpFx_l(\mathrm{TC}_k^{up} - T_l^{\mathrm{st}}) \\ \mathrm{TC}_k^{\mathrm{lo}} \leq T_l^{\mathrm{st}} \leq \mathrm{TC}_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{l,k}^{\mathrm{cx}_3} \\ Q_{l,k}^{\mathrm{cx}} = cpFx_l(\mathrm{TC}_k^{\mathrm{up}} - \mathrm{TC}_k^{\mathrm{lo}}) \\ T_l^{\mathrm{st}} \leq \mathrm{TC}_k^{\mathrm{lo}} \end{bmatrix} \end{bmatrix} \quad \forall l,\ \forall k \in \mathrm{CM} \tag{12}$$

$$\begin{bmatrix} Y_{m,k}^{\mathrm{ws}_1} \\ Q_{m,k}^{\mathrm{ws}} = cpFw_m(\mathrm{TC}_k^{\mathrm{up}} - \mathrm{TC}_k^{\mathrm{lo}}) \\ T_m^{\mathrm{ed}} \geq \mathrm{TC}_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{m,k}^{\mathrm{ws}_2} \\ Q_{m,k}^{\mathrm{ws}} = cpFw_m(T_m^{\mathrm{ed}} - \mathrm{TC}_k^{\mathrm{lo}}) \\ \mathrm{TC}_k^{\mathrm{lo}} \leq T_m^{\mathrm{ed}} \leq \mathrm{TC}_k^{\mathrm{up}} \end{bmatrix} \vee \begin{bmatrix} Y_{m,k}^{\mathrm{ws}_3} \\ Q_{m,k}^{\mathrm{ws}} = 0 \\ T_m^{\mathrm{ed}} \leq \mathrm{TC}_k^{\mathrm{lo}} \end{bmatrix} \quad \forall m,\ \forall k \in \mathrm{WM} \tag{13}$$

The following logic propositions are also needed for a complete description of the aforementioned alternatives

$$Y_l^{\mathrm{hx}} \veebar Y_l^{\mathrm{cx}} \quad \forall l \in \mathrm{MS} \tag{14}$$

$$Y_l^{\mathrm{hx}} \iff Y_{l,k}^{\mathrm{hx}_1} \veebar Y_{l,k}^{\mathrm{hx}_2} \veebar Y_{l,k}^{\mathrm{hx}_3} \quad \forall l,\ \forall k \in \mathrm{HM} \tag{15}$$

$$Y_l^{\mathrm{cx}} \iff Y_{l,k}^{\mathrm{cx}_1} \veebar Y_{l,k}^{\mathrm{cx}_2} \veebar Y_{l,k}^{\mathrm{cx}_3} \quad \forall l,\ \forall k \in \mathrm{CM} \tag{16}$$

$$Y_{m,k}^{\mathrm{ws}_1} \veebar Y_{m,k}^{\mathrm{ws}_2} \veebar Y_{m,k}^{\mathrm{ws}_3} \quad \forall m,\ \forall k \in \mathrm{WM} \tag{17}$$

Using binary variables, disjunctions (11–13) can be rewritten with the aid of Big-M formulation. Note that in disjunctions (11–13) equalities can be considered as a set of inequality constraints (i.e., $h(x)=0$ can be expressed as two inequality constraints: $h(x) \leq 0$ and $h(x) \geq 0$). For hot mixed stream, disjunction (11) is reformulated as follows

$$T_l^{\mathrm{st}} > T_l^{\mathrm{ed}} - M_1(1 - y_l^{\mathrm{hx}}) \tag{18}$$

$$\left.\begin{aligned} Q_{l,k}^{\mathrm{hx}_1} &\leq cpFx_l(\mathrm{TH}_k^{\mathrm{up}} - \mathrm{TH}_k^{\mathrm{lo}}) + M_2(1 - y_{l,k}^{\mathrm{hx}_1}) \\ Q_{l,k}^{\mathrm{hx}_1} &\geq cpFx_l(\mathrm{TH}_k^{\mathrm{up}} - \mathrm{TH}_k^{\mathrm{lo}}) - M_2(1 - y_{l,k}^{\mathrm{hx}_1}) \\ T_l^{\mathrm{st}} &\geq \mathrm{TH}_k^{\mathrm{up}} - M_1(1 - y_{l,k}^{\mathrm{hx}_1}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \mathrm{HM} \tag{19}$$

$$\left.\begin{aligned} Q_{l,k}^{\mathrm{hx}_2} &\leq cpFx_l(T_l^{\mathrm{st}} - TH_k^{\mathrm{lo}}) + M_3(1 - y_{l,k}^{\mathrm{hx}_2}) \\ Q_{l,k}^{\mathrm{hx}_2} &\geq cpFx_l(T_l^{\mathrm{st}} - TH_k^{\mathrm{lo}}) - M_3(1 - y_{l,k}^{\mathrm{hx}_2}) \\ TH_k^{\mathrm{lo}} &\leq T_l^{\mathrm{st}} + M_1(1 - y_{l,k}^{\mathrm{hx}_2}) \\ T_l^{\mathrm{st}} &\leq \mathrm{TH}_k^{\mathrm{up}} + M_1(1 - y_{l,k}^{\mathrm{hx}_2}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \mathrm{HM} \tag{20}$$

$$\left.\begin{aligned} Q_{l,k}^{\mathrm{hx}_3} &\leq M_2(1 - y_{l,k}^{\mathrm{hx}_3}) \\ T_l^{\mathrm{st}} &\leq TH_k^{\mathrm{lo}} + M_1(1 - y_{l,k}^{\mathrm{hx}_3}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \mathrm{HM} \tag{21}$$

$$\left.\begin{aligned} Q_{l,k}^{w} &\leq M_2 y_{j,k}^{w} \\ Q_{l,k}^{\mathrm{hx}} &= \sum_w Q_{l,k}^{w} \end{aligned}\right\} \quad \forall l,\ \forall k \in \mathrm{HM},\ \forall w \in \{\mathrm{hx}_1, \mathrm{hx}_2, \mathrm{hx}_3\} \tag{22}$$

In Eqs. 19–21, three disaggregated variables, $Q_{l,k}^{w}$, $w \in \{\mathrm{hx}_1, \mathrm{hx}_2, \mathrm{hx}_3\}$ are introduced to represent the heat exchange of hot mixed stream in temperature interval k. If $y_{l,k}^{w}=1$, then

Table 2. Boolean Variables to Model the Relative Positions of Streams to Temperature Intervals

Y_l^{hx}	True if mixed stream l is a hot stream
$Y_{l,k}^{\mathrm{hx}_1}$	True if the start temperature of hot mixed stream l is above temperature interval k
$Y_{l,k}^{\mathrm{hx}_2}$	True if the start temperature of hot mixed stream l is inside temperature interval k
$Y_{l,k}^{\mathrm{hx}_3}$	True if the start temperature of hot mixed stream l is below temperature interval k
Y_l^{cx}	True if mixed stream l is a cold stream
$Y_{l,k}^{\mathrm{cx}_1}$	True if the start temperature of cold mixed stream l is above temperature interval k
$Y_{l,k}^{\mathrm{cx}_2}$	True if the start temperature of cold mixed stream l is inside temperature interval k
$Y_{l,k}^{\mathrm{cx}_3}$	True if the start temperature of cold mixed stream l is below temperature interval k
$Y_{m,k}^{\mathrm{ws}_1}$	True if the end temperature of freshwater stream m is above temperature interval k
$Y_{m,k}^{\mathrm{ws}_2}$	True if the end temperature of freshwater stream m is inside temperature interval k
$Y_{m,k}^{\mathrm{ws}_3}$	True if the end temperature of freshwater stream m is below temperature interval k

$Q^{w}_{l,k}$ equals the value of heat exchanged by hot mixed stream in temperature interval k. Otherwise, $Q^{w}_{l,k}$ must be 0. To this end, Eq. 22 is added so that when $y^{w}_{l,k}=1$, $Q^{w}_{l,k}$ is bounded between 0 and M_2 and if $y^{w}_{l,k}=0$, $Q^{w}_{l,k}$ is forced to be 0. Hence, the final heat exchanged by hot mixed stream in temperature interval k equals the sum of the three disaggregated variables (see Eq. 22). This strategy is also applied to cold mixed stream and freshwater stream.

Similarly, disjunction (12) for cold mixed stream is reformulated as follows

$$T^{st}_l \le T^{ed}_l + M_1(1-y^{cx}_l) \tag{23}$$

$$\left.\begin{aligned} Q^{cx_1}_{l,k} &\le M_2(1-y^{cx_1}_{l,k}) \\ T^{st}_l &\ge TC^{up}_k - M_1(1-y^{cx_1}_{l,k}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \text{CM} \tag{24}$$

$$\left.\begin{aligned} Q^{cx_2}_{l,k} &\le cpFx_l(TC^{up}_k - T^{st}_l) + M_3(1-y^{cx_2}_{l,k}) \\ Q^{cx_2}_{l,k} &\ge cpFx_l(TC^{up}_k - T^{st}_l) - M_3(1-y^{cx_2}_{l,k}) \\ TC^{lo}_k &\le T^{st}_l + M_1(1-y^{cx_2}_{l,k}) \\ T^{st}_l &\le TC^{up}_k + M_1(1-y^{cx_2}_{l,k}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \text{CM} \tag{25}$$

$$\left.\begin{aligned} Q^{cx_3}_{l,k} &\le cpFx_l(\text{TC}^{up}_k - \text{TC}^{lo}_k) + M_2(1-y^{cx_3}_{l,k}) \\ Q^{cx_3}_{l,k} &\ge cpFx_l(\text{TC}^{up}_k - \text{TC}^{lo}_k) - M_2(1-y^{cx_3}_{l,k}) \\ T^{st}_l &\le TC^{lo}_k - M_1(1-y^{cx_3}_{l,k}) \end{aligned}\right\} \quad \forall l,\ \forall k \in \text{CM} \tag{26}$$

$$\left.\begin{aligned} Q^{w}_{l,k} &\le M_2 y^{w}_{l,k} \\ Q^{cx}_{l,k} &= \sum_w Q^{w}_{l,k} \end{aligned}\right\} \quad \forall l,\ \forall k \in \text{CM},\ \forall w \in \{\text{cx}_1, \text{cx}_2, \text{cx}_3\} \tag{27}$$

For freshwater stream, disjunction (13) is reformulated as follows

$$\left.\begin{aligned} Q^{ws_1}_{m,k} &\le cpFw_m(\text{TC}^{up}_k - \text{TC}^{lo}_k) + M_2(1-y^{ws_1}_{m,k}) \\ Q^{ws_1}_{m,k} &\ge cpFw_m(\text{TC}^{up}_k - \text{TC}^{lo}_k) - M_2(1-y^{ws_1}_{m,k}) \\ T^{ed}_m &\ge TC^{up}_k - M_1(1-y^{ws_1}_{m,k}) \end{aligned}\right\} \quad \forall m,\ \forall k \in \text{WM} \tag{28}$$

$$\left.\begin{aligned} Q^{ws_2}_{m,k} &\le cpFw_m(T^{ed}_m - TC^{lo}_k) + M_3(1-y^{ws_2}_{m,k}) \\ Q^{ws_2}_{j,k} &\ge cpFw_m(T^{ed}_m - TC^{lo}_k) - M_3(1-y^{ws_2}_{m,k}) \\ TC^{lo}_k &\le T^{ed}_m + M_1(1-y^{ws_2}_{m,k}) \\ T^{ed}_m &\le TC^{up}_k + M_1(1-y^{ws_2}_{m,k}) \end{aligned}\right\} \quad \forall m,\ \forall k \in \text{WM} \tag{29}$$

$$\left.\begin{aligned} Q^{ws_3}_{m,k} &\le M_2(1-y^{ws_3}_{m,k}) \\ T^{ed}_m &\le TC^{lo}_k + M_1(1-y^{ws_3}_{m,k}) \end{aligned}\right\} \quad \forall m,\ \forall k \in \text{WM} \tag{30}$$

$$\left.\begin{aligned} Q^{w}_{m,k} &\le M_2 y^{w}_{m,k} \\ Q^{ws}_{m,k} &= \sum_w Q^{w}_{m,k} \end{aligned}\right\} \quad \forall m,\ \forall k \in \text{WM},\ \forall w \in \{\text{ws}_1, \text{ws}_2, \text{ws}_3\} \tag{31}$$

As the relative positions of wastewater stream to each temperature interval are known, heat exchanged by wastewater stream in temperature interval k is computed directly by Eq. 32

$$Q^{ww}_{n,k} = cpWw_n[min\{T^{st}_n, \text{TH}^{up}_k\} - min\{T^{st}_n, \text{TH}^{lo}_k\}] \tag{32}$$

The logic propositions (Eqs. 14–17) can be converted into linear inequality constraints

$$y^{hx}_l + y^{cx}_l = 1 \quad \forall l \in \text{MS} \tag{33}$$

$$y^{hx}_l = y^{hx_1}_{l,k} + y^{hx_2}_{l,k} + y^{hx_3}_{l,k} \quad \forall l,\ \forall k \in \text{HM} \tag{34}$$

$$y^{cx}_l = y^{cx_1}_{l,k} + y^{cx_2}_{l,k} + y^{cx_3}_{l,k} \quad \forall l,\ \forall k \in \text{CM} \tag{35}$$

$$y^{ws_1}_{m,k} + y^{ws_2}_{m,k} + y^{ws_3}_{m,k} = 1 \quad \forall m,\ \forall k \in \text{WM} \tag{36}$$

As hot and cold mixed streams and freshwater streams cannot appear in temperature intervals that do not belong to HM, CM, and WM, we can write the following constraints

$$y^{w}_{l,k}=0,\ Q^{w}_{l,k}=0 \quad \forall w \in \{\text{hx}_1, \text{hx}_2, \text{hx}_3\},\ \forall l,\ \forall k \notin \text{HM} \tag{37}$$

$$y^{w}_{l,k}=0,\ Q^{w}_{l,k}=0 \quad \forall w \in \{\text{cx}_1, \text{cx}_2, \text{cx}_3\},\ \forall l,\ \forall k \notin \text{CM} \tag{38}$$

$$y^{w}_{m,k}=0,\ Q^{w}_{m,k}=0 \quad \forall w \in \{\text{ws}_1, \text{ws}_2, \text{ws}_3\},\ \forall m,\ \forall k \notin \text{WM} \tag{39}$$

The total heat supplied by hot streams to temperature interval k and the total heat removed by cold streams from temperature interval k are calculated as follows

$$Q^{hs}_k = \sum_{l,n}(Q^{hx}_{l,k} + Q^{ww}_{n,k}) \quad \forall l \in \text{MS},\ \forall n \in \text{WWS},\ k=1,2,...,K \tag{40}$$

$$Q^{cs}_k = \sum_{l,m}(Q^{cx}_{l,k} + Q^{ws}_{m,k}) \quad \forall l \in \text{MS},\ \forall m \in \text{FWS},\ k=1,2,...,K \tag{41}$$

In transshipment model, as shown Figure 3, the energy balance for each temperature interval k may be expressed as follows

$$R_k - R_{k-1} - Q^{HU}_k + Q^{CU}_k = Q^{hs}_k - Q^{cs}_k \quad k=1,2,...,K \tag{42}$$

As no streams exist above the highest temperature interval or below the lowest temperature interval, residual heat flow constraints can be written as

$$R_0 = R_K = 0 \tag{43}$$

Non-negative constraints are expressed as

$$\left.\begin{aligned} &Fw_j, F_{i,j}, Fx_j, Ww_j, Tw_j, Tx_j, Qp_j, Qn_j, T^{st}_l, T^{ed}_m, Q^{hx_1}_{l,k}, Q^{hx_2}_{l,k}, Q^{hx_3}_{l,k}, Q^{hx}_{l,k} \\ &Q^{cx_1}_{l,k}, Q^{cx_2}_{l,k}, Q^{cx_3}_{l,k}, Q^{cx}_{l,k}, Q^{ws_1}_{m,k}, Q^{ws_2}_{m,k}, Q^{ws_3}_{m,k}, Q^{ws}_{m,k}, Q^{ww}_{n,k}, Q^{hs}_{n,k}, Q^{cs}_{n,k}, Q^{HU}_k, Q^{CU}_k, R_k \end{aligned}\right\} \ge 0 \tag{44}$$

Table 3. Cost and Operating Parameters for Example 1

Parameter		Parameter		Parameter	
CHU	260 $\$\cdot kW^{-1}$	CCN	3000 \$	*tcui*	15°C
CCU	150 $\$\cdot kW^{-1}$	h (process stream and cold utility)	1 $kW\cdot m^{-2}\cdot K^{-1}$	*tcuo*	20°C
CF	10000 \$	h (hot utility)	5 $kW\cdot m^{-2}\cdot K^{-1}$	*thui*	126°C
CA	860 $\$\cdot m^{-2}$	B	0.75	*thuo*	126°C
CFW	2.5 $\$\cdot t^{-1}$	fa	0.95	ΔT_{min}	10°C

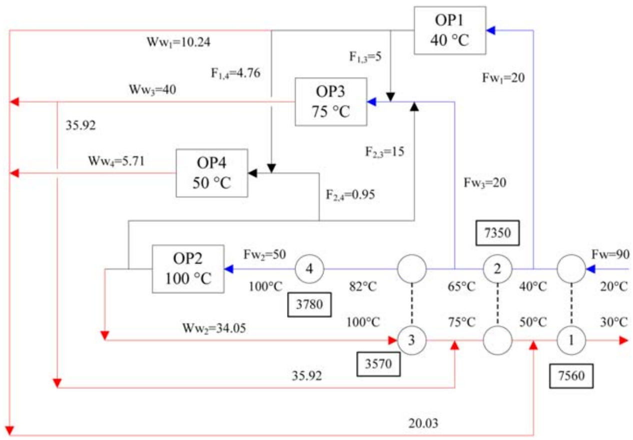

Figure 6. Optimal WAHEN of Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 4. Heat Load and Heat Exchanger Area of Example 1

Heat Exchanger Number	1	2	3	4
Heat load (kW)	7560	7350	3570	3780
Area (m^2)	1512	1470	524.6	132.6

$$y_l^{hx}, y_l^{cx}, y_{l,k}^{hx_1}, y_{l,k}^{hx_2}, y_{l,k}^{hx_3}, y_{l,k}^{cx_1}, y_{l,k}^{cx_2}, y_{l,k}^{cx_3}, y_{m,k}^{ws_1}, y_{m,k}^{ws_2}, y_{m,k}^{ws_3} = 0, 1 \tag{45}$$

Objective function

The objective function of the model is the annual operational cost of WAHEN, composed of cost terms for freshwater and hot and cold utilities. It can be seen that, with such an objective function, the minimization of the utility cost may tend to be achieved by increasing the nonisothermal mixing (see Eq. 6), which may lead to the increase of the number of streams, and then the investment cost and operation issues. To avoid the complexity of involving such complex factor into the model, we introduce here a weight parameter to manipulate the extent of the utility cost related to the nonisothermal mixing. Then, the objective function is written as

$$\min z = \text{fa}\left(N_h \text{CFW}\sum_j Fw_j + \text{CHU}\sum_k Q_k^{HU} + \text{CCU}\sum_k Q_k^{CU}\right) + a\sum_j (Qp_j + Qn_j) \tag{46}$$

where a is a price parameter, which acts as the weight parameter. In the solutions of the example problems in this article, we run the calculation a number of time with different values of a to find a proper one so that the increase in the number of streams can be kept reasonable. As such, the tradeoff among freshwater usage, utility consumption and nonisothermal mixing can be achieved.

Herein, the GDP model is transformed into MINLP model, which comprises of Eqs. GDP–10 and 18–46. We call this MINLP model **MP**. WAHEN is designed based on the optimal WAN obtained by solving **MP**. On the basis of the optimal WAN, a detailed HEN to satisfy the targeted utility consumption is then synthesized. This new method is employed to synthesize WAHEN for simultaneous minimization of water and energy consumption in the following section.

Examples

Three examples from literature, including two large-scale problems, are given in this section to illustrate the advantages and applicability of the proposed method. The examples are implemented in GAMS[29] and solved using BARON with CPLEX as the MIP solver and MINOS as the NLP solver. Solving **MP** results in an optimal WAN that realizes simultaneous integration of water and energy while maximizing the direct heat transfer by nonisothermal mixing. Based on the optimal WAN, a detailed HEN to satisfy the targeted

Table 5. Results Comparison of Example 1

Items	Ref. 7	Ref. 22	Ref. 24	Ref. 23	Ref. 20	Our Method
Freshwater ($kg\cdot s^{-1}$)	90	90	90	90	90	90
Hot utility (kW)	3780	3780	3780	3780	3780	3780
Cold utility (kW)	0	0	0	0	0	0
Number of streams[a]	7	7	-	16	-	7
Heat exchanger unit	4	4	5	4	3	4
Heat exchanger area (m^2)	3638.4	3645.0	3912.6	3495.9	3823.2	3639.2
Annual water cost (M\$)	6.741	6.741	6.741	6.741	6.741	6.741
Annual energy cost (M\$)	0.933	0.933	0.933	0.933	0.933	0.933
Capital cost (M\$)	0.617	0.624	0.668	0.601	0.549	0.617
Total annual cost (M\$)	8.291	8.298	8.342	8.275	8.223	8.291

[a]Number of streams for HEN design.
- Not reported in the literature.

Table 6. Data for Example 2

Process Number	Mass Load of Contaminant (g s^{-1})	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	2	25	80	40
2	2.88	25	90	100
3	4	25	200	80
4	3	50	100	60
5	30	50	800	50
6	5	400	800	90
7	2	400	600	70
8	1	0	100	50

Temperature of freshwater source T_{ws}=20°C.
Temperature of wastewater T_{ww}=30°C.

utility consumption can be synthesized adequately using the principles of pinch design method[30] with proper stream mixing. After the final network structure is obtained, the areas of heat exchangers in HEN and the total annual cost of WAHEN are calculated. In order to compare our results with those published in literature, our cost and operating parameters are used to recalculate costs (water cost, energy cost, capital cost, and finally total annual cost) of the optimal designs reported in literature for the three examples. The results comparison shows that our method presents a reasonable and effective strategy for WAHEN synthesis and is applicable for large-scale problems.

Example 1

The first example includes four water-using units with process data shown in Table 1. Its cost and operating parameters are adopted from Bogataj and Bagajewicz,[22] and listed in Table 3.

By solving **MP**, an optimal WAN is obtained with the minimum freshwater usage (90 kg·s^{-1}) and hot utility consumption (3780 kW). These targets are the same as those obtained by Leewongtanawit and Kim,[7] Bogataj and Bagajewciz,[22] Liao et al.,[23] Dong et al.,[24] and Ahmetovic and Kravanja.[20] Three freshwater streams and four wastewater streams are obtained for HEN design. The optimal WAHEN is shown in Figure 6, from which we can see that one heater and three heat exchangers are used to achieve the minimum utility consumption. These numbers also agree with the results of Leewongtanawit and Kim,[7] Bogataj and Bagajewciz,[22] and Liao et al.[23] Heat load and area of each heat exchanger are listed in Table 4. The detailed results comparison with other works is presented in Table 5.

As shown in Table 5, these results are close. That means our method is as effective as those published by other groups for simple problems such as Example 1. However, the studies of large-scale problems are seldom reported. So far, for single contaminant problems, only two examples in the literature are larger than Example 1. One is offered by Bagajewicz et al.[15] while the other is provided by Luo et al.[13] To show the advantages and applicability of our method, we solve these two problems in the following Example 2 and Example 3, respectively.

Example 2

The second example is a large system from Bagajewicz et al.[15] The system is composed of eight water-using units and their data are presented in Table 6. The cost and operating parameters for this example are taken from Liao et al.[23]

Table 7. Cost and Operating Parameters for Example 2

Parameter		Parameter		Parameter	
CHU	136.8 \$·kW^{-1}	CFW	1500 \$·h·t^{-1}	*tcui*	15°C
CCU	12.6 \$·kW^{-1}	U	0.86 kW·m^{-2}·K^{-1}	*tcuo*	20°C
			2.2 kW·m^{-2}·K^{-1} (heater)	*thui*	120°C
CF	8600 \$	B	0.6	*thuo*	120°C
CA	1200 \$·m^{-2}	fa	1	ΔT_{min}	10°C

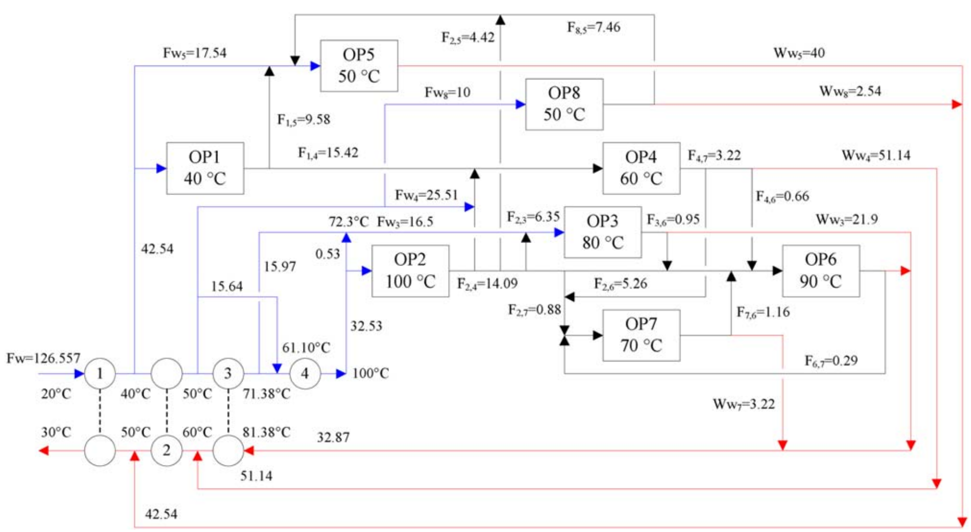

Figure 7. Optimal WAHEN of Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 8. Heat Load and Heat Exchanger Area of Example 2

Heat Exchanger Number	1	2	3	4
Heat load (kW)	10630.8	3528.6	2951.6	5315.38
Area (m^2)	1236.14	410.30	343.21	67.20

Table 9. Results Comparison of Example 2

Items	Ref. 15 (case b)	Ref. 23 (case b)	Ref. 23 (case a)	Our Method (case a)
Freshwater ($kg{\cdot}s^{-1}$)	125.94	125.94	127.713	126.557
Hot utility (kW)	5290	5290	5363.94	5315.38
Cold utility (kW)	0	0	0	0
Number of streams[a]	22	39	32	12
Heat exchanger unit	12	8	4	4
Heat exchanger area (m^2)	2111.69	1341.76	2008.18	2056.85
Annual water cost (k$)	680.1	680.1	689.6	683.4
Annual energy cost (k$)	723.6	723.6	733.8	727.1
Capital cost (k$)	403.0	279.2	218.3	219.6
Total annual cost (k$)	1806.7	1682.9	1641.7	1630.1

[a]Number of streams for HEN design.

and shown in Table 7. An optimal WAN where the integration of water and energy is accomplished in one step is derived from applying **MP** to Example 2. The minimum freshwater, hot utility and cold utility consumptions are 126.557 kg s^{-1}, 5315.38 kW, and 0 kW, respectively. The resulting streams for HEN design are six freshwater streams and six wastewater streams. Figure 7 shows the optimal WAHEN containing three heat exchangers and one heater, while the heat load and area of each heat exchanger are presented in Table 8. The WAHEN has a capital cost of 219.6 k$ and a total annual cost of 1630.1 k$.

Liao et al.[23] considered this example in two cases: case a, a uniform treating of wastewater; case b, separate treating of wastewater. Our method treats wastewater in a uniform way. Comparisons with the works of Bagajewciz et al.[15] and Liao et al.[23] are summarized in Table 9. As can be seen, our freshwater and utility consumption is less than those obtained by Liao et al.[23] in case a. This is because nonisothermal mixing of streams is fully made use of in our work. Furthermore, the number of streams for HEN design in our work is far less than that of Bagajewciz et al.[15] and Liao et al.,[23] suggesting that our HEN design is much easier. In other words, our method could greatly reduce the complexity of subsequent HEN design. Finally, our design has a lower total annual cost compared with the design of Bagajewciz et al.[15] and Liao et al.[23] Although the minimum freshwater and utility consumption is obtained in case b, more heat exchangers are required to achieve the targeted utility consumption. This will definitely result in higher capital cost and total annual cost than case a, as shown in Table 9. Therefore, we could conclude that our design is the best in terms of total annual cost. Furthermore, the final network structure obtained by our method is much simpler than the ones reported by Bagajewicz et al.[15] and Liao et al.[23]

Table 10. Data for Example 3

Process Number	Mass Load of Contaminant ($g\ s^{-1}$)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	1	0	100	50
2	2	0	100	80
3	4	0	200	110
4	4.5	0	300	90
5	0.5	0	100	100
6	2	250	400	70
7	2.25	150	300	100
8	1.5	200	250	120
9	1	300	350	80
10	1.8	350	380	95
11	1	300	350	110
12	1.2	350	400	95
13	6	0	200	100
14	0.3	380	400	100
15	0.8	350	380	60

Temperature of freshwater source T_{ws}=30°C
Temperature of wastewater T_{ww}=30°C.

Table 11. Cost and Operating Parameters for Example 3

Parameter		Parameter		Parameter	
CHU	388 $\${\cdot}kW^{-1}$			tcui	10°C
CCU	189 $\${\cdot}kW^{-1}$	U	0.5 $kW{\cdot}m^{-2}{\cdot}K^{-1}$	tcuo	20°C
CF	8000 $	B	0.6	thui	150°C
CA	1200 $\${\cdot}m^{-2}$	fa	0.95	thuo	150°C
CFW	0.375 $\${\cdot}t^{-1}$			ΔT_{min}	10°C

Example 3

The third example is adopted from Luo et al.[13] and consists of 15 water-using units. This example is the largest in the existing literature and no studies of WAHEN synthesis have been reported so far. The data are illustrated in Table 10 while the cost and operating parameters are presented in Table 11. By solving **MP**, the minimum freshwater, hot utility and cold utility consumptions are determined to be 100 kg s^{-1}, 4200 kW, and 4200 kW, respectively. These targets are achieved by one-step optimization. Six freshwater streams, one cold mixed stream, and eight wastewater streams are employed to design HEN. The optimal network structure is shown in Figure 8. There are one cooler, six heat exchangers and two heaters in HEN, whose heat loads and heat exchanger areas are presented in Table 12. The capital cost and total annual cost of this example are 492.9 k$ and 3918.6 k$, respectively. The detailed results are shown in Table 13.

If we solved this example by the method of Liao et al.,[23] the number of streams for network design would increase to 60 in case a and to 74 in case b, respectively. This leads to an exponential increase in model size and makes the problem very difficult to solve. However, in our work, only 15 streams are considered for HEN design, as shown in Table 13, which greatly reduces the complexity of HEN design and makes the HEN much simpler. Hence, our method is effective for simultaneous integration of water and energy in large-scale WAHEN systems.

Conclusion

We propose a new methodology in this article for simultaneous integration of water and energy in WAHEN. A novel GDP model is first developed to determine an optimal WAN which realizes simultaneous integration of water and energy while maximizing nonisothermal mixing of streams. Based

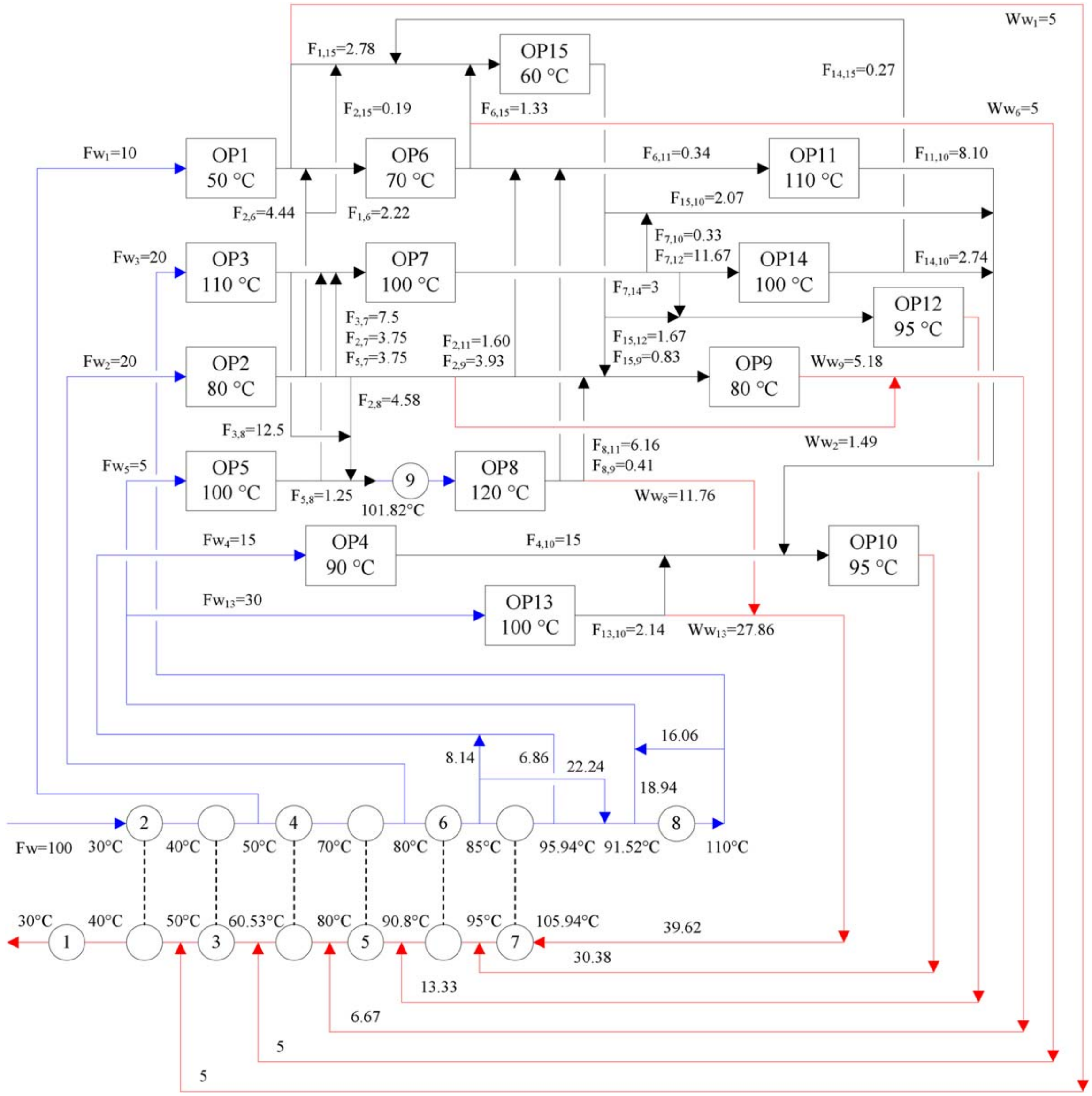

Figure 8. Optimal WAHEN of Example 3.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

on the optimal WAN, a detailed HEN to satisfy the utility target is then synthesized. In this method, the optimal targets of freshwater and utility are obtained in one step.

Our method has three distinct advantages. First of all, it can capture a tradeoff among freshwater usage, utility consumption and direct heat transfer by nonisothermal mixing. Second, it can greatly reduce the complexity of subsequent HEN design. Finally, it is effective for simultaneous integration of water and energy in large-scale WAHEN systems. This is highly valuable from an industrial application point of view.

Three examples, including two large-scale problems have been analyzed in this article. Our results are almost the same

Table 12. Heat Load and Heat Exchanger Area of Example 3

Heat Exchanger Number	Heat load (kW)	Area (m^2)
1	4200	420
2	4200	840
3	4200	818.47
4	3780	756
5	3780	726.92
6	1470	294
7	1820.5	364.1
8	2800	115.08
9	1400	72.97

Table 13. Optimal Results of Example 3

Items	Our Results
Freshwater ($kg \cdot s^{-1}$)	100
Hot utility (kW)	4200
Cold utility (kW)	4200
Number of streams[a]	15
Heat exchanger unit	9
Heat exchanger area (m^2)	4407.54
Annual water cost (k$)	1123.5
Annual energy cost (k$)	2302.2
Capital cost (k$)	492.9
Total annual cost (k$)	3918.6

[a]Number of streams for HEN design.

as or better than those obtained by other researchers through different methods, which testifies the effectivity of our method. Currently, the proposed method could only be applied to achieve simultaneous integration of water and energy. In the future, it will be modified to synthesize both WAN and HEN by one-step optimization, which will be presented in our next work.

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Notation

Indices

i, j = water-using unit
l = mixed stream
m = freshwater stream
n = wastewater stream
k = temperature interval

Sets

P = set of water-using units
MS = set of mixed streams
FWS = set of freshwater streams
WWS = set of wastewater streams
HM = set of temperature interval where hot mixed stream may be located
CM = set of temperature interval where cold mixed stream may be located
WM = set of temperature interval where freshwater stream may be located

Parameters

B = exponent for area cost
C = contaminant concentration, ppm
CA = area cost coefficient, $\$\cdot m^{-2}$
CCU = cost of cold utility, $\$\cdot kW^{-1}$
CF = fixed cost for heat exchangers, \$
CFW = cost of freshwater, $\$\cdot t^{-1}$
CHU = cost of hot utility, $\$\cdot kW^{-1}$
cp = stream heat capacity, kJ kg^{-1} K^{-1}
fa = time fraction of operation
h = stream heat transfer coefficient, $kW\cdot m^{-2}\cdot K^{-1}$
K = total number of temperature intervals
L = mass load of contaminant, $g\cdot s^{-1}$
M_1, M_2, M_3 = big-M parameters
N_h = number of hours per year, h
T = operating temperature of water-using unit, °C
ΔT_{min} = minimum approach temperature, °C
T_{ws} = temperature of freshwater source, °C
T_{ww} = temperature of wastewater, °C
T^{max} = maximum operating temperature, °C
TC_k = the kth cold temperature boundary, °C
TC_k^{lo} = lower boundary of temperature interval k at cold side, °C
TC_k^{up} = upper boundary of temperature interval k at cold side, °C
$tcui$ = inlet temperature of cold utility, °C
$tcuo$ = outlet temperature of cold utility, °C
TH_k = the kth hot temperature boundary, °C
TH_k^{lo} = lower boundary of temperature interval k at hot side, °C
TH_k^{up} = upper boundary of temperature interval k at hot side, °C
$thui$ = inlet temperature of hot utility, °C
$thuo$ = outlet temperature of hot utility, °C
U = overall heat transfer coefficient, $kW\cdot m^{-2}$ K^{-1}

Continuous, non-negative variables

F = flow rate of reused water stream, kg s^{-1}
Fx = flow rate of mixed stream, kg s^{-1}
Fw = flow rate of freshwater, kg s^{-1}
Q_k^{HU} = heat supplied by hot utility in temperature interval k, kW
Q_k^{CU} = heat removed by cold utility in temperature interval k, kW
$Q_{l,k}^{hx}$ = heat supplied by hot mixed stream l to temperature interval k, kW
$Q_{l,k}^{cx}$ = heat removed by cold mixed stream l from temperature interval k, kW
$Q_{m,k}^{ws}$ = heat removed by freshwater stream m from temperature interval k, kW
$Q_{n,k}^{ww}$ = heat supplied by wastewater stream n to temperature interval k, kW
Q_k^{hs} = heat content of hot streams in temperature interval k, kW
Q_k^{cs} = heat content of cold streams in temperature interval k, kW
Qn, Qp = heat demand of mixed stream, kW
R_k = heat residual of temperature interval k, kW
T^{st} = start temperature of water stream, °C
T^{ed} = end temperature of water stream, °C
Tx = start temperature of mixed stream, °C
Tw = end temperature of freshwater stream, °C
Ww = flow rate of wastewater, kg s^{-1}

Binary variables

y_l^{hx} = 1 if mixed stream l is a hot stream
$y_{l,k}^{hx_1}$ = 1 if the start temperature of hot mixed stream l is above temperature interval k
$y_{l,k}^{hx_2}$ = 1 if the start temperature of hot mixed stream l is inside temperature interval k
$y_{l,k}^{hx_3}$ = 1 if the start temperature of hot mixed stream l is below temperature interval k
y_l^{cx} = 1 if mixed stream l is a cold stream
$y_{l,k}^{cx_1}$ = 1 if the start temperature of cold mixed stream l is above temperature interval k
$y_{l,k}^{cx_2}$ = 1 if the start temperature of cold mixed stream l is inside temperature interval k
$y_{l,k}^{cx_3}$ = 1 if the start temperature of cold mixed stream l is below temperature interval k
$y_{m,k}^{ws_1}$ = 1 if the end temperature of freshwater stream m is above temperature interval k
$y_{m,k}^{ws_2}$ = 1 if the end temperature of freshwater stream m is inside temperature interval k
$y_{m,k}^{ws_3}$ = 1 if the end temperature of freshwater stream m is below temperature interval k

Subscripts/Superscripts

CU = cold utility
cs = cold streams
cx = cold mixed stream
ed = end temperature
HU = hot utility
hs = hot streams
hx = hot mixed stream
in = inlet of water-using unit
lo = lower boundary
max = maximum
out = outlet of water-using unit
st = start temperature
up = upper boundary
ws = freshwater
ww = wastewater

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