Int. J. Environ. Res., 4(1):11-26,Winter 2010
ISSN: 1735-6865

Simultaneous Energy and Water Optimization in Multiple-Contaminant Systems with Flowrate Changes Consideration

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Received 7 Nov. 2008; Revised 16 Aug. 2009; Accepted 25 Aug. 2009

ABSTRACT: In this paper, a new systematic design methodology has been developed for the simultaneous energy and water minimization in multiple-contaminant systems that also feature maximum re-use of water. In addition to allowing re-use of water in multiple-contaminant systems, issues about heat losses and flowrate changes inside unit operations have also been incorporated in this new design method. To implement such a design, two new design aspects are introduced; new method for "Non-isothermal Mixing" point identification and new "Separate System" generation. The first aspect involves "non-isothermal mixing", which enables direct heat recovery between water streams, and therefore allows the reduction of the number of heat transfer units. The other aspect is the generation of "separate system "in heat exchanger network design. The flexibility of mixing and splitting of water streams allows separate systems to be created as a cost-effective series of heat-exchanger units between freshwater and wastewater streams. The new design aspects have been illustrated with two examples.

Key word: Heat loss, Non-isothermal mixing, Separate system, Heat recovery, Heat-exchanger network

INTRODUCTION

Water is one of the most widely used raw materials in chemical and petroleum industries. Significant amounts of water are required in washing, stripping, and manufacturing processes. As water resources face scarcities, ever-increasing prices, and more stringent environmental regulations, much attention has been paid to reduce freshwater consumption and wastewater generation (Kim & Smith, 2002), (Ataei *et al.*, 2009d) There are conceptual and automated approaches as two traditional methods to design water networks with re-use of water (Panjeshahi and ataei, 2008). The former analysis exploits graphical tools to explore the possibilities of water reuse, whilst the latter employs mathematical optimization models to obtain a cost-effective solution (Alva-Argaez, 1999), (Ataei *et al.*, 2009c). The analysis of water management generally involves water distribution among water-using operations with the criteria of contaminant concentration levels (Mann & Liu, 1999).

In some cases such as sterilization and process-washing, temperature of water becomes as important as the quality of water (Bagajewicz *et al.*, 2002). The water system is now subject to not only the constraints of contaminant concentration levels, but also those of the temperature levels. Water streams need to be heated up or cooled down to satisfy the temperature requirements of the operations and energy consumption become necessary for these heating and cooling tasks (Smith, 2005). Under these circumstances, energy and water management needs to be considered simultaneously. Therefore, the problem has become a combined analysis of water and energy systems (see Fig. 1).

The simultaneous energy and water minimization was first addressed by Savulescu

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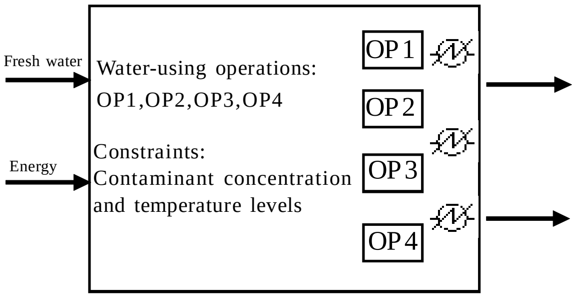

Fig.1. Simultaneouse water and energy management

(1999). In this methodology, several assumptions are made for problem simplification but these assumptions make the design inaccurate. Some of these assumptions are:

- Each water-using operation has a fixed temperature and runs isothermally.
- The water flowrate through an operation does not change.
- Only single contaminant operations are considered.

It should be noted that for particular operations, temperature of water changes and hence isothermally running assumption for practical water-using operations cannot be correct. Furthermore, in industrial practices, many water-using operations have fixed flowrate requirements, such as in many vessel-cleaning operations (Young *et al.*, 2006). Also, there may be a fixed flowrate of water loss (e.g., cooling-tower evaporation) or gain (e.g., dewatering filter). Accordingly, the flowrate changes should be considered in design of water-using networks with minimum water and energy consumption. Savulescu design considers only the networks with single contaminant and the non-isothermal mixing point identification is based on water-pinch analysis and synthesis. Therefore, extension of this method for multiple contaminant problems may be tedious. Accordingly, An NLP model should be formulated to identify feasible non-isothermal mixing points, which satisfy minimum freshwater and utility requirements in both of single and multiple contaminant problems. Two main stages are suggested for simultaneous water and energy minimization through Savulescu methodology:
Stage 1: Two dimensional grid diagram for designing a water network.
Stage 2: Separate system approach for designing a heat exchanger network.

This method is a sequential approach that follows a set of design rules in the first stage, to provide a water network with less heat exchanger units required. These rules, however, do not always guarantee minimum utility requirement. In other words, the actual utility requirement of the design is higher than the utility target and the design with small number of heat exchangers could be obtained but with utility penalty. Furthermore, in the presented design method, temperature of some water streams in the network may increase to above the normal boiling temperature. This temperature increasing can cause many operational problems for the process; however, increasing of the process pressure, which suggested in this method, cannot be a no-cost and easy solution for these problems.In the second stage, the idea of generating separate systems to simplify a heat exchanger network design was introduced. Nevertheless, the generation of separate systems has not been fully explored from the recognition that a smaller number of heat exchanger units could be acquired. Moreover, the optimum heat transfer area in each separate system should be explored by introducing a trade-off between the capital cost of heat exchanger and the power losses because of the pressure drops of each fluid to achieve minimum total annual cost. Accordingly, a new methodology should be developed to construct a water structure without the utility penalty and the increasing of water streams temperature to above the normal boiling point, and provide a heat exchanger network with minimum number of units and optimum heat transfer area.This paper addresses the simultaneous management of energy and water as an approach for multiple-contaminant systems with maximum re-use of water. In addition, the heat loss and water flowrate changes through operations have been considered in this new methodology. In other words, In addition to overcome the aforementioned limitations of Savulecsu design method, the simplifier assumptions of it have been relaxed in this new simultaneous water and energy minimization approach.The new simultaneous water and energy minimization technique has been tested through two illustrative examples. Related coding in GAMS optimization package was used for illustrative examples to get optimal values in the proposed design method computations.

MATERIALS & METHODS

The new systematic design methodology has been developed for the simultaneous management of energy and water in multiple-contaminant systems that also feature maximum re-use of water. In addition to allowing re-use of water, issues about heat losses and water flowrate changes inside unit operations have also been incorporated in this design method. The general features of the problem involve a set of water-using operations with specifications of flowrates, temperature and contaminant concentration levels, a selection of water sources with different qualities, and a number of heat transfer units. It is desired to determine water and energy targets and specify the distribution of water among the water-using operations as well as the allocation of heat exchangers between these water streams in order to complete the overall network configuration.The new design method comprises two new design aspects; new method for "Non-isothermal Mixing" point identification to design a water network with the minimum freshwater and energy requirements and new "Separate System" generation for designing a heat exchanger network with minimum number of heat exchanger units and optimum heat transfer area. Moreover, in the proposed method, the optimum detail design of the heat exchanger related to each separate system can be achieved. Fig. 2 shows an example of the non-isothermal mixing area and separate systems in the cold and hot composite curves.

New Method for "Non-Isothermal Mixing" Point Identification

Non-isothermal mixing enables direct heat recovery between water streams, and therefore allows the reduction of the number of heat transfer units. However, non-isothermal mixing can cause the degradation of temperature driving forces, and also reduces the number of possibilities of indirect heat transfer matching between hot and cold streams (Baldyga *et al.*, 1998). Thus, in the introduction of non-isothermal mixing, a water network without utility penalty should be considered.

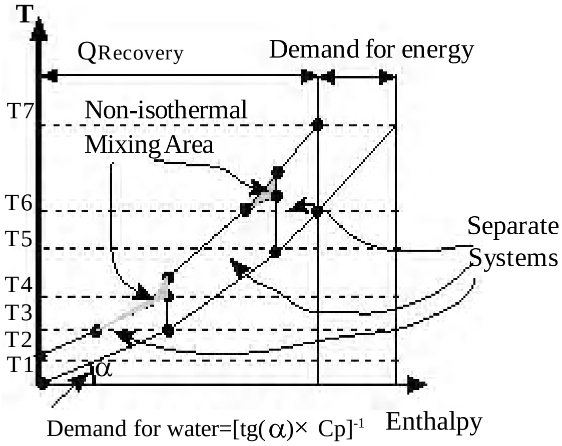

Fig. 2. "Non-isothermal Mixing" area and "Separate Systems" in the composite curves

In this study, an NLP model is formulated to identify feasible non-isothermal mixing points, which satisfy not only the inlet requirements (temperature and contaminant concentration levels) of the operations but also achieve the minimum freshwater and utility requirements and create an overall water network with fewer number of heat exchanger units. By using this mathematical model, the water network design with small number of heat exchangers and minimum operating cost can be obtained without utility penalty. Fig. 3 depicts a general water-using operation i . Here, we define the operation with a fixed mass load of contaminant $j(j=1,2,3,\ldots,n_{contaminants})$, to be transferred, $\Delta m_{i,j,tot}$, and with maximum allowable concentrations of contaminant $j(j=1,2,3,\ldots,n_{contaminants})$ at the inlet, $C_{i,j,in}^{\max}$, and outlet, $C_{i,j,out}^{\max}$, of the operation. We include inlet streams from the freshwater source at temperature T_0 and heated to T_{fi} with a flowrate, $f_i(i=1,2,3,\ldots,n_{operations})$, as well as streams reused from other operations, $k(k=1,2,3,\ldots,n_{operations})$, at a flowrate, $X_{i,k}$, temperature of $T_{k,out}$ and a contaminant $j(j=1,2,3,\ldots,n_{contaminants})$ concentration, $C_{k,j,out}$. Likewise, we consider an outlet stream to wastewater treatment at a flowrate, W_i, temperature of $T_{i,out}$ and a contaminant $j(j=1,2,3,\ldots,n_{contaminants})$ concentration, $C_{i,j,out}$,and outlet streams for reuse in other operations,

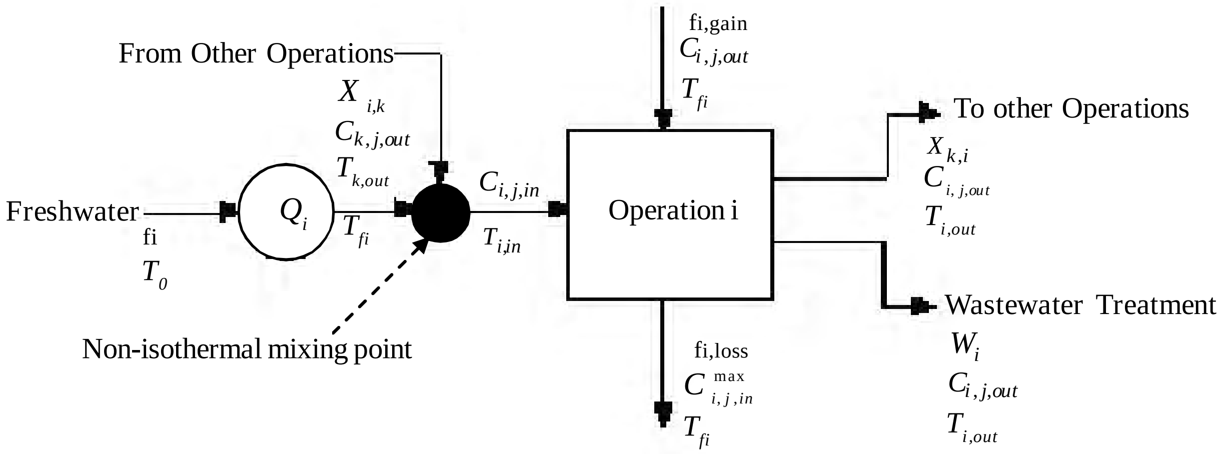

Fig. 3. Illustration of the NLP model for non-isothermal mixing point identification in a multiple-contaminant system with flowrate changes consideration

$k(k=1,2,3,\ldots,n_{operations})$ at flowrates, $X_{k,i}$, temperature of $T_{i,out}$ and concentration of contaminant $j(j=1,2,3,\ldots,n_{contaminants})$, $C_{i,j,out}$.

The total operating cost, as the objective function, is expressed in Eq. (1) (Ataei *et al.*, 2009a);

$$Min\ OPCOST = C_W \sum_{i=1}^{n_{operations}} f_i + C_e \sum_{i=1}^{n_{operations}} Q_i \tag{1}$$

We formulate the constraints governing water reuse from the maximum inlet and outlet concentrations as well as the fixed mass load of contaminants transferred in each operation. We calculate the average inlet concentration of contaminant j, $C_{i,j,in}$, by the flowrate-weighted average of the concentrations provided by the fresh water source and reused from other operations;

$$C_{i,j,in} = \frac{\sum_{k\neq i} X_{i,k} C_{k,j,out}}{\sum_{k\neq i} X_{i,k} + f_i} \leq C^{\max}_{i,j,in} \tag{2}$$

We relate the outlet concentration of contaminant j from operation i, $C_{i,j,out}$, to $C_{i,j,in}$ and the change in concentration due to the fixed mass load of contaminant j transferred, $\Delta m_{i,j,tot}$, as follows:

$$C_{i,j,out} = C_{i,j,in} + \frac{\Delta m_{i,j,tot}}{\sum_{k\neq i} X_{i,k} + f_i} = C^{\max}_{i,j,out} \tag{3}$$

Substituting for $C_{i,in}$ from Eq. (2) into Eq. (3) gives;

$$C_{i,j,out} = \frac{\sum_{k\neq i} X_{i,k} C_{k,j,out} + \Delta m_{i,j,tot}}{\sum_{k\neq i} X_{i,k} + f_i} = C^{\max}_{i,j,out} \tag{4}$$

By re-arranging Eqs. (3) and (4), a set of more linear constraints can be formed as follows;

$$\sum_{k\neq i} [C^{\max}_{i,j,in} - C_{k,j,out}] X_{i,k} + C^{\max}_{i,j,in} f_i \geq 0 \tag{5}$$

$$\sum_{k\neq i} [C^{\max}_{i,j,out} - C_{k,j,out}] X_{i,k} + C^{\max}_{i,j,out} f_i = \Delta m_{i,j,out} \times 10^3 \tag{6}$$

In addition, we include a mass balance on water around each operation i as follows;

$$f_i + \sum_{j\neq i} X_{i,j} - W_i - \sum_{j\neq i} X_{j,i} = 0 \tag{7}$$

We specify that all concentrations and flowrates be positive. The temperature of inlet water stream to the operation i, $T_{i,in}$ and the temperature of outlet water stream from the operation i, $T_{i,out}$, are fixed and known parameters. The constraint related to the fixed and known amount of inlet water temperature can be expressed as Eq. (8);

$$T_{i,in}\left[\left(\sum_{j\neq i} X_{i,j}\right) + f_i \right] = \left[\left(\sum_{j\neq i} T_{j,out} X_{i,j}\right) + T_{fi} f_i \right] \tag{8}$$

The energy requirement for heating of the inlet freshwater to the operation i from temperature T_0 to T_{fi} is given by Eq.(9);

$$Q_i = Kf_i C_p (T_{fi} - T_o) \qquad (9)$$

The nonlinear program to optimize the water-using network, without water flowrate changes consideration, is to minimize the total operating cost, *OPCOST* expressed in Eq. (1), subject to Eqs. (5), (6), (7), (8) and (9).As we develop constraints for mathematical optimization, we have a greater freedom to tailor our model for the type of water-using operations involved. For non-isothermal mixing point identification in water networks with water flowrate changes, (water gain, water loss and fixed water flowrate), the presented NLP model should be revised.For a water gain, we can formulate the constraints governing water reuse from the maximum inlet and outlet concentrations as well as the fixed mass load of contaminant j transferred in each operation just as in Eqs. (5) and (6). However, we include an increase in the flowrate through operation i, $f_{i,gain}$. The mass balance on water around each operation i with only a water gain becomes;

$$f_i + \sum_{k \neq i} X_{i,k} + f_{i,gain} - W_i - \sum_{k \neq i} X_{k,i} = 0 \qquad (10)$$

When Eq. (10) is included in place of Eq. (7) as a mass balance on water, the optimization procedure will make an additional flowrate of $f_{i,gain}$ available for reuse from operation i. Equations (5) and (6) remain valid as the constraints on the limiting inlet and outlet concentrations for operation i, respectively. In this condition, the constraints governing inlet and outlet water temperatures as well as fresh water heating from temperature T_0 to T_{fi} just as in Eqs. (11) and (12). Therefore, Eqs. (11) and (12) should be included in place of Eqs.(8) and (9).

$$T_{i,in}\left[\left(\sum_{j \neq i} X_{i,j}\right) + f_i + f_{i,gain}\right] = \left[\left(\sum_{j \neq i} T_{j,out} X_{i,j}\right) + T_{fi}\left(f_i + f_{i,gain}\right)\right] \qquad (11)$$

$$Q_i = K\left(f_i + f_{i,gain}\right)C_p (T_{fi} - T_o) \qquad (12)$$

However, if we wish to include a water loss at the limiting inlet concentration of contaminant j, we must modify both constraints on the limiting inlet and outlet concentrations as well as the water balance. The average inlet concentration of contaminant j, $C_{i,j,in}$, is given by the flowrate-weighted average of the concentrations from all other operations and the freshwater. Note that the numerator contains a term, $f_{i,loss} C_{i,j,in}^{\max}$, to account for a water loss at the limiting inlet concentration of contaminant j, to operation i;

$$C_{i,j,in} = \frac{\sum_{k \neq i} X_{i,k} C_{k,j,out} - f_{i,loss} C_{i,j,in}^{\max}}{\sum_{k \neq i} X_{i,k} + f_i - f_{i,loss}} \leq C_{i,j,in}^{\max} \qquad (13)$$

The outlet concentration is the sum of the average inlet concentration of contaminant j, $C_{i,j,in}$, and the change in concentration of contaminant j due to the fixed mass load of contaminant j transferred, $\Delta m_{i,j}^{fixed}$ by only the flowrate of water that passes completely through the operation;

$$C_{i,j,out} = C_{i,j,in} + \frac{\Delta m_{i,j,out}}{\sum_{k \neq i} X_{i,k} + f_i - f_{i,loss}} = C_{i,j,out}^{\max} \qquad (14)$$

Substituting for $C_{i,j,in}$ from Eq. (13) into Eq. (14) gives;

$$C_{i,j,out} = \frac{\sum_{k \neq i} X_{i,k} C_{k,j,out} - f_{i,loss} C_{i,j,in}^{\max} + \Delta m_{i,j,out}}{\sum_{k \neq i} X_{i,k} + f_i - f_{i,loss}} = C_{i,j,out}^{\max} \qquad (15)$$

We rearrange Eqs.(14) and (15) to form another linear constraint as follows;

$$\sum_{k \neq i} [C_{i,j,out}^{\max} - C_{k,j,out}] X_{i,k} + C_{i,j,out}^{\max} f_i - f_{i,loss} [C_{i,j,out}^{\max} - C_{i,j,in}^{\max}] = \Delta m_{i,j,out} \times 10^3 \qquad (16)$$

In addition, we form a mass balance on water around each operation i;

$$f_i + \sum_{k \neq i} X_{i,k} - f_{i,loss} - W_i - \sum_{k \neq i} X_{i,k} = 0 \qquad (17)$$

Equations (8) and (9) remain valid as the constraints on the inlet water temperature to operation i and heating of the inlet fresh water to operation i from temperature T_0 to T_{fi}, respectively.We may choose to model an operation i with a fixed flowrate (f_i^{fixed}) while maintaining maximum inlet and outlet concentrations. A water balance across the operation gives;

$$f_i + \sum_{k \neq i} X_{i,k} = W_i + \sum_{k \neq i} X_{k,i} = f_i^{fixed} \qquad (18)$$

Equations (5) and (6) remain applicable to the constraints on the inlet and outlet concentrations, respectively. Also Eqs. (8) and (9) remain valid as the constraints on the inlet water temperature to operation i and heating of the inlet fresh water to operation from temperature T_0 to T_{fi}, respectively.The presented NLP model can be a useful tool to determine water and energy targets and specify the distribution of water among the water-using operations with and without flowrate changes consideration.After the connections between operations are established by using the above mentioned model, heat exchanger network design is considered to complete the overall network configuration. In the next section, a new separate system approach will be introduced to design the heat exchanger network.

New Method for "Separate System" Generation

Once the non-isothermal mixing for the water re-use streams is completed, the remaining design is to identify the matching of water streams by generating separate systems and appropriate location of separate systems. The remaining problem of heat recovery involves only fresh water streams as cold streams and wastewater streams as hot streams, which enables a simple heat exchanger network design with fewer heat transfer units (Kim *et al.*, 2001). To design a cost-effective heat exchanger network for the water system, new separate system generation has been developed. As each separate system represents a heat transfer unit between hot and cold streams, the number of separate systems should be minimized in order to achieve the minimum number of heat exchanger units. Besides, the temperature driving forces in each separate system should be maximized to reduce heat transfer area (Savulescu *et al.*, 2002). Moreover, the optimum heat transfer area in each separate system should be explored by introducing a trade-off between the capital cost of heat exchanger and the cost related to compensation of pressure drops in tube and shell sides, for achieving the minimum total annual cost. Therefore, the concept of new separate system approach intends to create minimum number of separate systems and optimum heat transfer area in each separate system. The procedure of the new separate system approach is based on the five steps as follows:

Step 1; Construct the energy composite curves

The initial energy composite curves are generated based on individual thermal stream data extracted from the water network. As shown in Fig. 2. the minimum demand for fresh water can be targeted by the slope of the fresh water supply line from the cold composite curve. The energy target obtained from the analysis of these composite curves is the same as the value of energy consumption estimated in the stage of non-isothermal mixing point identification.

Step 2; Minimize the number of separate systems

In order to achieve the minimum number of separate systems and consequently fewer heat transfer units, separate systems should be generated following kink points on the composite curve with fewer kink points. Then, the boundaries of separate systems can be defined at kink points from the selected curve.

Step 3; Maximize temperature driving force in each separate system.

The creation of separate systems involves non-isothermal stream mixing in order to achieve the temperatures required by the water-using operations. Through non-isothermal mixing of hot wastewater streams, the hot composite curve should be modified to maintain maximum driving force in each separate system for reducing the heat transfer area.

Step 4; Determine water distribution between separate systems and operations

Since some modifications have been made to the composite curves, water distribution between the separate systems and the operations should be determined. The water distribution involving non-isothermal mixing of wastewater streams can be carried out by solving a simple series of mass and heat balance equations.

Step 5; Optimize heat transfer area in each separate system

After determination of cold and hot streams in each separate system in *step 4,* the optimum heat transfer area in each separate system should be explored by introducing a trade-off between the capital cost of heat exchanger and the cost related to compensation of pressure drops in the tube side and shell side, for achieving the minimum total annual cost.

Here we examine a procedure for optimizing the heat transfer area in each separate system. We assume the heat exchanger, which represented by each separate system, is a baffled shell-and-tube, single-pass, counter flow heat exchanger (Fig. 4). in which the tube fluid is in turbulent flow but no change of phase of fluids takes place in the shell or tubes. It should be noted that the inlet and outlet flowrates and temperatures to and from the tube side and shell side of the heat exchanger in each separate system are known in this stage (Edgar *et al.,* 2001). Also, the tube spacing and tube inside and outside diameters should be specified a priori by the designer (Nordman & Berntsson, 2001). Note that the presented optimization procedure is specified for a general separate system *j*. Thus, this procedure should be carried out for each of separate systems individually.The total cost of the heat exchanger in the separate system *j*, as the objective function in dollars per year, is formulated as follows (Ataei *et al.,* 2009c);

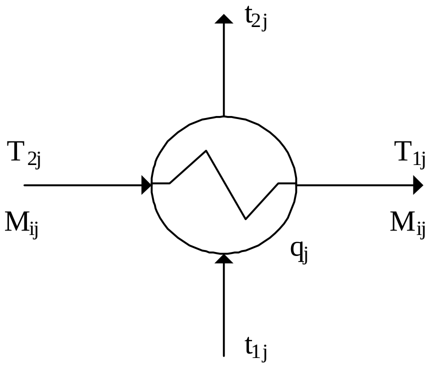

Fig. 4. Illustration of the NLP model for optimization of the heat transfer area in a general separate system j. (Key: $\Delta t_{1f} = T_{1f} - t_{1f}$ cold-end temperature difference; $\Delta t_{2f} = T_{2f} - t_{2f}$ warm-end temperature difference)

$$Min\,TC_j = A_{oj}\,(C_{Aj} + C_{ij}\,E_{ij} + C_{oj}\,E_{oj}) \qquad (19)$$

The rate of indirect heat transfer in the separate system j is given in Eq.(20) (Polley *et al.,* 1990);

$$q_j = F_{tj} U_{oj} A_{oj} \frac{\Delta t_{2j} - \Delta t_{1j}}{Ln\left(\frac{\Delta t_{2j}}{\Delta t_{1j}}\right)} \qquad (20)$$

F_{tj} is unity for a single-pass exchanger for the separate system j (Glavic, 2001). U_{oj} is given by the values of h_{oj}, h_{ij}, and the fouling coefficient h_{tj} in the separate system *j*, as follows (Polley & Panjeshahi, 1991);

$$\frac{1}{U_{oj}} = \frac{1}{f_{Aj} h_{ij}} + \frac{1}{h_{oj}} + \frac{1}{h_{tj}} \qquad (21)$$

h_{tj} is a combined coefficient for tube wall and dirt films, based on tube outside area. This parameter is expressed in Eq.(22) (Jarzebski *et al.,* 1977), (Ramalho &Alabastro, 1966);

$$\frac{1}{h_{tj}} = \frac{l'_j A_{oj}}{k_{wj} A_{lmj}} + \frac{A_{oj}}{h_{f_i j} A_{ij}} + \frac{1}{h_{f_o j}} \qquad (22)$$

Cichelli and Brinn (1956) showed that the annual pumping cost terms in Eq. (19) could be related to h_{ij} and h_{oj} by using friction factors for tube flow and shell flow;

$$E_{ij} = \varphi_{ij} h_{ij}^{3.5} \qquad (23)$$

$$E_{oj} = \varphi_{oj} h_{oj}^{4.75} \qquad (24)$$

The coefficients φ_{ij} and φ_{oj} depend on fluid specific heat, thermal conductivity, density and viscosity as well as the tube diameters in the separate system j. φ_{oj} is based on either in-line or staggered tube arrangements.If we substitute for E_{ij} , E_{oj} in Eq. (19), the resulting objective function can be expressed as Eq.(25) (Woods *et al.,* 1976);

$$Min\,TC_j = C_{Aj} A_{oj} + C_{ij} \varphi_{ij} h_{ij}^{3.5} A_{oj} + C_{oj} \varphi_{oj} h_{oj}^{4.75} A_{oj} \qquad (25)$$

To accommodate the constraint on the fixed and known indirect heat transfer rate in the separate system j, a Lagrangian function L_j is formed by augmenting TC_j with Eq. (26), using a Lagrange multiplier ω_j as follows (Ataei *et al.*, 2009a);

$$L_j = TC_j + \omega_j \left[\frac{F_{tj}\left(\Delta t_{2j} - \Delta t_{1j}\right)}{Q_j Ln\left(\frac{\Delta t_{2j}}{\Delta t_{1j}}\right)} - \frac{1}{U_{oj} A_{oj}} \right] \qquad (26)$$

Eq. (26) can be differentiated with respect to four variables $(h_{ij}, h_{oj}, \Delta t_{2j}\ and\ A_{oj})$. After some rearrangement, a relationship between the optimum h_{oj} and h_{ij} can be obtained as follows (McAdams, 1954);

$$h_{oj} = \left(\frac{0.74 C_{ij} \varphi_{ij} f_{Aj}}{C_{oj} \varphi_{oj}} \right)^{0.17} h_{ij}^{\ 0.78} \qquad (27)$$

The value of h_{ij} in the separate system j can be obtained by solving the following equation;

$$C_{Aj} - 2.5 C_{ij} \varphi_{ij} h_{ij}^{3.5} - 2.91 (C_{oj} \varphi_{oj})^{0.17} (C_{ij} \varphi_{ij} f_{Aj})^{0.83} h_{ij}^{3.72} - \frac{3.5 C_{ij} \varphi_{ij} f_{Aj} h_{ij}^{4.5}}{h_{tj}} = 0 \qquad (28)$$

Accordingly, the following algorithm can be used to obtain the optimal values of heat transfer coefficients, power loss inside and outside tubes because of pressure drops and heat transfer area in the separate system j without the explicit calculation of ω_j;

I.Solve for h_{ij} from Eq. (28).

II.Obtain h_{oj} from Eq. (27).

III.Calculate U_{oj} from Eq. (21).

IV.Determine E_{ij} and E_{oj} from h_{ij} and h_{oj} using Eqs. (23) and (24).

V.Calculate A_{oj} from Eq. (20).

Note that steps I to V require that several nonlinear equations be solved one at a time.

Optimal Detail Design of the Heat Exchanger Related to Each Separate System

Once the optimal four variables (h_{ij}, h_{oj}, Δt_{2i}, *and* A_{oj}) were calculated in the previous stage, the physical dimensions of the heat exchanger in each separate system can be determined. Accordingly, the following algorithm can be used to obtain the optimal detail design of the heat exchanger related to each separate system;

I. Determine the optimal v_{ij} and v_{oj} from h_{ij} and h_{oj} using the appropriate heat transfer correlations (McAdams, 1954); recall that the inside and outside tube diameters are specified a priori.

II. The number of tubes N_{tj} can be found from a mass balance as follows;

$$v_{ij} N_{tj} \frac{\pi D_{ij}^{2}}{4} = KM_{ij} \qquad (29)$$

III. The length of the tube can be found from Eq. (30);

$$A_{oj} = N_{tj} \pi D_{oj} L_{tj} \qquad (30)$$

IV. The number of clearances can be found from N_{tj} based on either square pitch or equilateral pitch. The flow area S_{oj} is obtained from v_{oj} (flow normal to a tube bundle). Finally, baffle spacing (or the number of baffles) is computed from S_{oj}, A_{oj}, N_{tj} and N_{cj}.

N_{tj} N_{cj}

RESULTS & DISCUSSION

The application of the new simultaneous water and energy minimization technique presented in this paper is demonstrated on two different examples. The design specifications for both of examples have been given in Table 1. As presented in Table 1. the temperature of the fresh water supply in these examples is assumed to be fixed (20 °C) and the effluent discharge temperature is assumed to be 30°C. Therefore, heat can be recovered from the effluent until ΔT_{min} (10 °C) is achieved.

Example 1

The first example is a multiple-contaminant problem without water flowrate changes but with heat loss inside unit operations. The limiting water-using operations data of example 1 are given in

Table 2. Applying the new NLP model to illustrative example 1, through the commercial mathematical optimization software package GAMS, an optimum water network, which can achieve both minimum freshwater (70 t/h) and hot utility (1983.3 kW) consumption, is identified in Fig. 5.

Table 1. Design specifications of examples 1 and 2

Process specifications and economical data	
Fresh water supply temperature, °C	20
Environmental temperature discharge limit, °C	30
Specific heat capacity for water and wastewater streams, kJ/kg°C	4.2
Cost of fresh water, $/t	0.26
Cost of hot utility, $/kWh	0.005
Cost of cold utility, $/kWh	0.000625
Cost of supplying 1 kW electricity to pump shell side fluid, $/kWh	0.05
Cost of supplying 1 kW electricity to pump tube side fluid, $/kWh	0.05
Annual cost of heat exchanger per unit outside tube surface area, $/m^{2}yr	385
Payback time, yr	4
Hours operation per year, h/yr	8000
Interest rate, %	15
Design specifications for heat exchangers	
Fouling resistance in shell and tube sides, m^{2}°C/W	0.00018
Tube material	Carbon steel
Type of tube layout	Triangular
Construction type	Fixed tube sheet
Maximum allowable shell diameter, mm	1000
Number of tube passes	1
Tube outside diameter, mm	19.05
Tube thickness, mm	2.11

As shown in Fig. 5, the network includes two non-isothermal mixing points (direct heat transfer). One is the mixing of a freshwater stream and a reuse stream at the inlet of Operation 2. The other is the mixing of a freshwater stream and a reuse stream at the inlet of Operation 3. These mixings can reduce the number of heat exchanger units required in the design without non-isothermal mixing. The targeting results for example 1 are given in Table 3. After the connections between operations are created, design of heat exchanger network through the new separate system approach is considered to complete the optimum overall network configuration. The thermal data of streams referred to the optimum water network (Fig. 5) are given in Table 4.

The initial energy composite curves based on the thermal stream data and a minimum temperature approach (10 °C) which indicates the minimum water and energy requirements in the new water network (example 1) are shown in Fig. 6. As represented in Fig. 6, these composite curves assure that the energy requirements in the new water network achieve the utility target to 1983.3 kW hot utility and 0 kW cold utility.To achieve the minimum number of separate systems in example 1, separate systems are created following kink points on the cold composite curve. Then, the boundaries of separate systems can be defined at kink points from the cold composite curve as shown in Fig. 6. In addition, the hot composite curve is modified to maintain maximum driving force in each separate system. Heat loads exchanged between wastewater and freshwater streams in the separate systems are vertically transferred, and the shaded areas between the original and the modified hot composite curves represent the non-isothermal mixing points of hot wastewater streams from operations.

According to Fig. 6. by applying the new separate system generation method to example 1, only two heat exchangers represented by two separate systems can be enough to complete overall network configuration.The optimum heat transfer area and detail design for each heat exchanger related to the represented separate systems are found by the introduced trade-off between the capital cost of heat exchanger and the cost related to compensation of pressure drops in the tube side and shell side. Fig. 7 illustrates the effect of the heat transfer area on the total annual cost of heat exchangers 1 and 2 related to the represented separate systems in example 1. The optimum heat transfer area achieves the minimum total annual cost. The optimum design of heat exchangers 1 and 2 has been given in Table 5. In example 1, the total number of heat transfer units is three, as there are two heat exchangers (separate systems) plus one heater. The new and conventional network configurations for example 1 is presented in Fig. 8.

Table 2. The operating data of example 1

Operation *i*	**Contaminant *j***	$\Delta m_{i,j,out}$	$C_{i,j,in}^{max}$	$C_{i,j,out}^{max}$	**Inlet temperature**	**Outlet temperature**
		kg/h	**ppm**	**ppm**	**^oC**	**^oC**
Operation *1*	A	3	0	100	90	80
	B	2.4	0	80		
	C	1.8	0	60		
Operation *2*	A	4	50	150	50	40
	B	3	40	115		
	C	3.6	15	105		
Operation *3*	A	1.5	50	125	85	70
	B	0.6	50	80		
	C	2	30	130		

Table 3. The targeting results for example 1

Targeted requirements	
Fresh water, t/h	70
Hot utility, kW	1983.3
Cold utility, kW	0
Annual cost of fresh water, $/yr	145600
Annual cost of hot utility, $/yr	79333
Annual cost of cold utility, $/yr	0
Total annual cost of operating , $/yr	224933

Table 4. Thermal steam data from the water network of Fig. 5.

Streams	**Inlet temperature (^oC)**	**Outlet temperature (^oC)**	**Heat flow capacity (kW/^oC)**	**Enthalpy (kW)**
Freshwater to operation 1 and a mixing point	20	90	46.6667	3266.669
Freshwater to a mixing point	20	40	35	700
Wastewater from operation 1	80	30	11.6667	583.335
Wastewater from operation 2	40	30	46.6667	466.667
Wastewater from operation 3	70	30	23.3333	933.332

Table 5. Optimum design of heat exchangers 1 and 2 for example 1

HEX 1	Number of shell in series	1	Tube counts	112
	Number of shell in parallel	1	Number of tube passes	1
	Shell diameter, mm	384	Tube layout	30
	Tube thickness, mm	2.11	Baffle cut, %	45
	Tube outside diameter, mm	19.05	Baffle spacing, mm	450
	Tube pitch, mm	25	Baffle type	Single segmental
	Tube length, m	2.438	Area, m^2	16.33
HEX 2	Number of shell in series	1	Tube counts	73
	Number of shell in parallel	1	Number of tube passes	1
	Shell diameter, mm	315	Tube layout	30
	Tube thickness, mm	2.11	Baffle cut, %	45
	Tube outside diameter, mm	19.05	Baffle spacing, mm	450
	Tube pitch, mm	25	Baffle type	Single segmental
	Tube length, m	2.438	Area, m^2	10.65

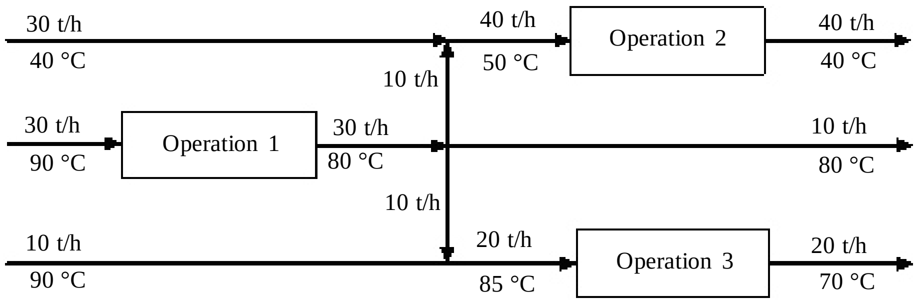

Fig. 5. An optimum water network for example 1

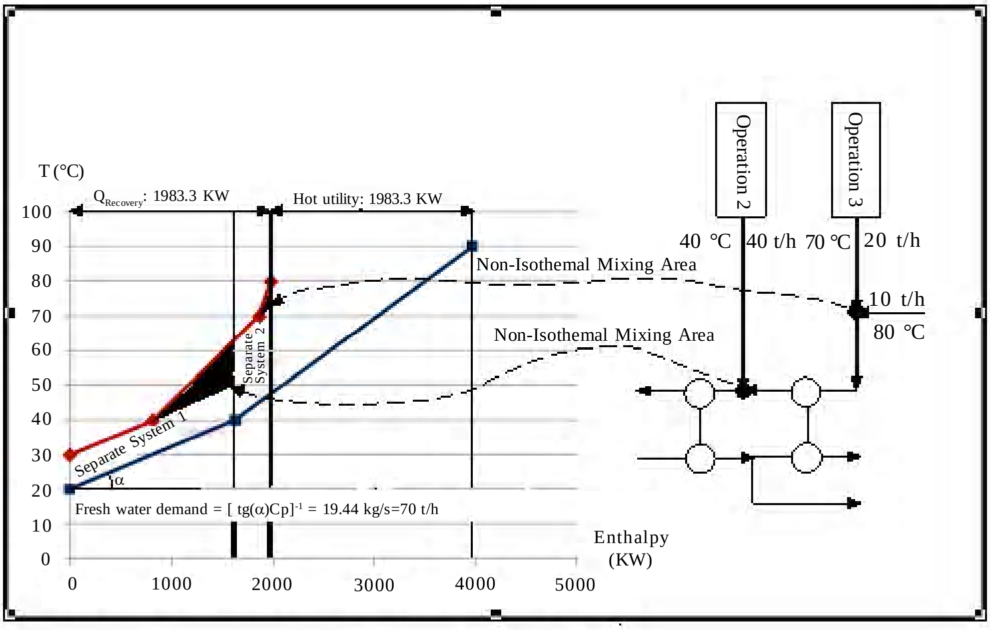

Fig. 6. New separate system approach for example 1

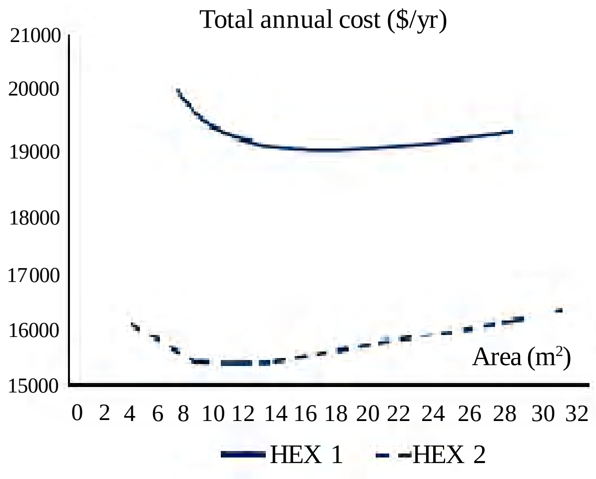

Fig. 7. Total annual cost of heat exchangers 1 and 2 related to the represented separate systems in example 1

Example 2

The second example is a multiple-contaminant problem with heat loss inside unit operations and with water loss in operations 1 & 5, water gain in operation 3 and water fixed flowrate in operations 2 & 4. The limiting water-using operations data of example 2 are given in Table 6.Formulating and solving the presented NLP model to illustrative example 2, through the GAMS optimization software, an optimum water network, which can achieve both minimum freshwater (93.02 t/h) and hot utility (4923.1 kW) consumption, is shown in Fig. 9. The targeting results for example 2 are given in Table 7.

After the connections between operations are created, optimum design of heat exchanger network can be achieved similar to example 1. In other words, only formulation of the presented NLP model for non-isothermal mixing point

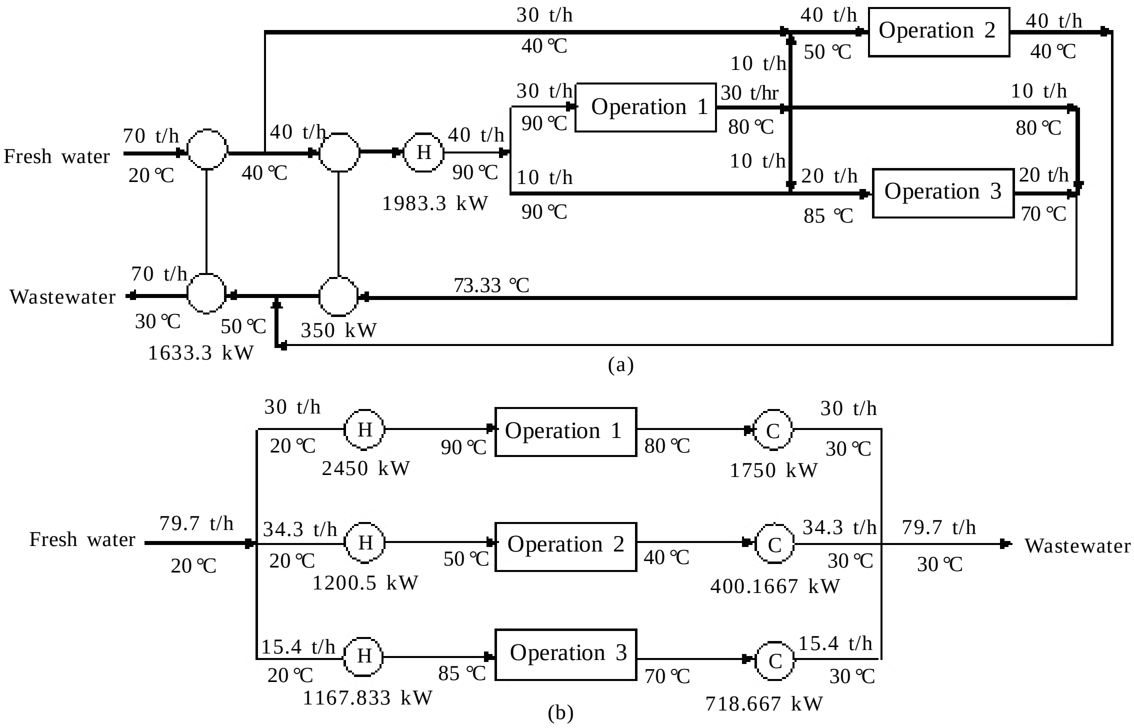

Fig. 8. (a) New network configuration, (b) Conventional network configuration for example 1

Table 6. The operating data of example 2

Operation *i*	**Contaminant *j***	$C_{i,j,in}^{\max}$	$C_{i,j,out}^{\max}$	$f_{i,in}^{\lim}$	$f_{i,out}^{\lim}$	**Inlet temperature**	**Outlet temperature**
		ppm	**ppm**	**t/h**	**t/h**	**°C**	**°C**
Operation 1	A B	100 10	1000 100	80	20	92	80
Operation 2	A B	300 200	800 700	50	50	78	75
Operation 3	A B	0 0	0 0	10	40	95	80
Operation 4	A B	0 0	0 0	10	10	75	60
Operation 5	A B	10 10	100 50	15	5	65	60

Table 7. The targeting results for example 2

Targeted requirements	
Fresh water, t/h	93.02
Hot utility, kW	4923.1
Cold utility, kW	0
Annual cost of fresh water, $/yr	193482
Annual cost of hot utility, $/yr	196924
Annual cost of cold utility, $/yr	0
Total annual cost of operating , $/yr	390406

identification is different between example 1 and example 2, but the method for separate systems generation and optimum design of heat exchangers are the same in both of examples. The new and conventional network configurations for example 2 are presented in Fig.10.As shown in Fig. 10. the total number of heat transfer units for example 2 is three, as there are two heaters plus one heat exchanger (separate system). A comparison of designs from the conventional and new approaches for examples 1 and 2 is made in Table 8. As presented in Table 8. the new approach provides a better design with less utility usage, fewer heat transfer units and smaller total annual cost for both of examples.

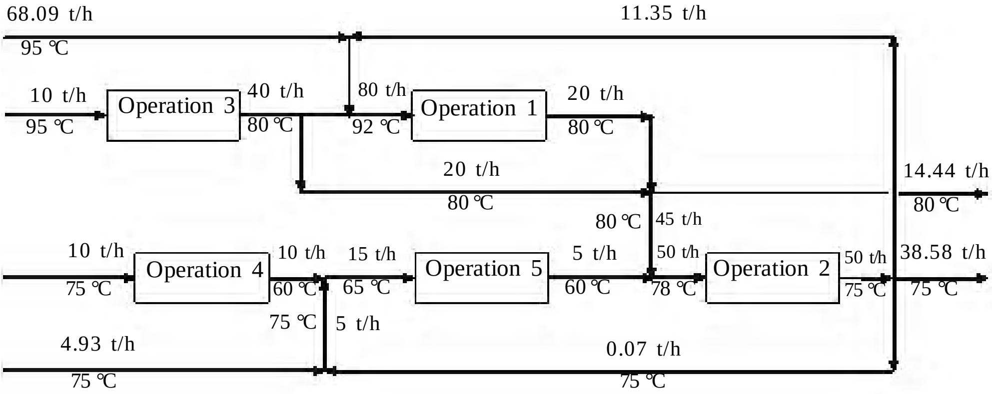

Fig. 9. An optimum water network for example 2

Table 8. The result comparison for both of examples

	Requirements	New design	Conventional design	Saving, %
Example 1	Fresh water, t/h	70	79.7	12.2
	Hot utility, kW	1983.3	4818.3	58.8
	Cold utility, kW	0	2869	100
	Number of heat transfer units	3	6	50
	Total annual cost, $/yr	259333	474853	45.4
Example 2	Fresh water, t/h	93.02	165	43.6
	Hot utility, kW	4923.1	12407.5	60.3
	Cold utility, kW	0	6650	100
	Number of heat transfer units	3	10	70
	Total annual cost, $/yr	409793	1066750	61.6

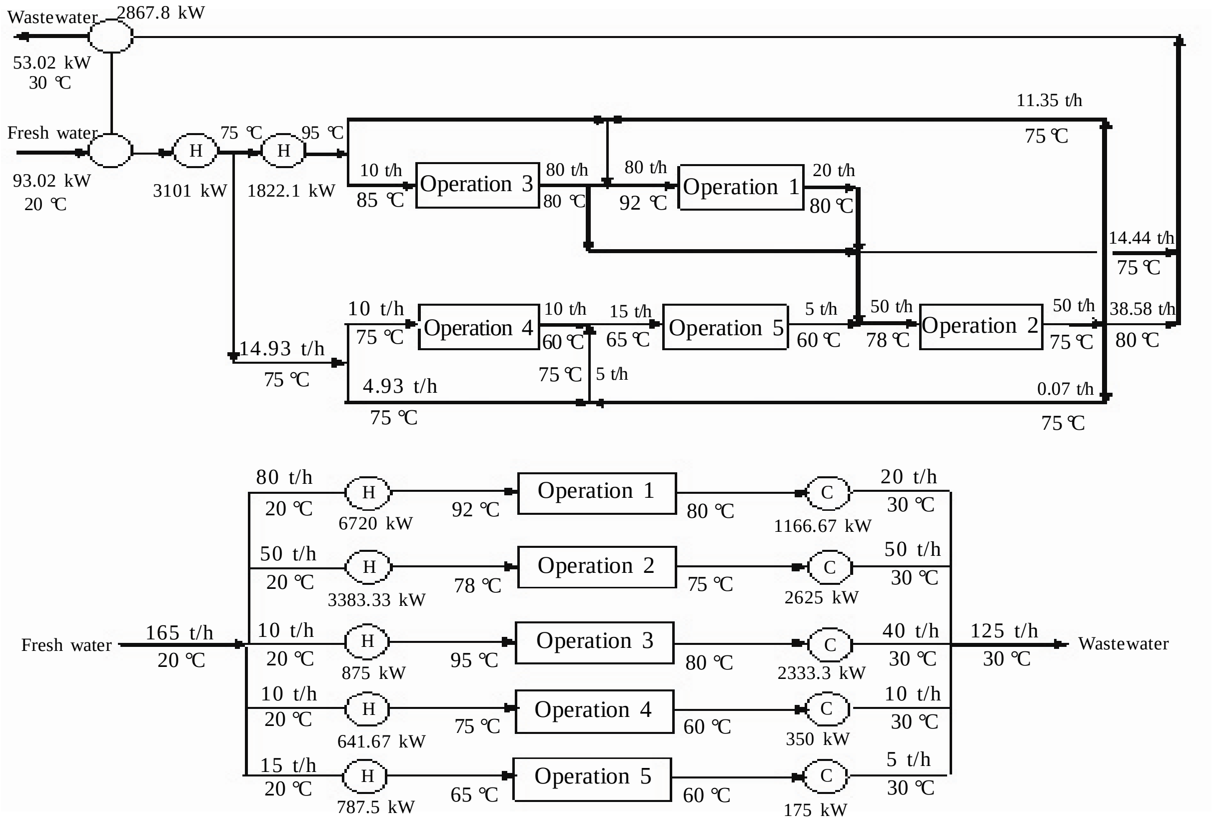

Fig. 10. (a) New network configuration, (b) Conventional network configuration for example 2

CONCULSION

Process integration has been highlighted in this paper to provide a new systematic design methodology for the problem of simultaneous energy and water minimization in multiple-contaminant systems with consideration of flowrate changes and heat losses inside unit operations.

The method relies on two sequential design aspects to achieve the water and energy targets; new method for non-isothermal mixing points identification and new separate system generation. In the new method for non-isothermal mixing point's identification, reuse options of water within the water-using systems with multiple-contaminant are exploited not only from the point of view of contaminant concentration, but also considering energy. An NLP model is proposed to identify feasible non-isothermal mixing points, which create an overall water network with minimum freshwater and utility consumption. Then, new separate system generation is developed to design a simplified heat exchanger network. The new approach provides a heat exchanger network with fewer heat transfer units and optimal heat transfer area.

The presented simultaneous water and energy minimization technique has been tested through two multiple-contaminant examples that one of those was with water flowrate changes. Optimization was made using the commercial mathematical optimization software package GAMS. The results of the analysis for example 1 demonstrated 12.2% of fresh water, 58.8% of hot utility, 100% of cold utility, 50% of number of heat transfer units and 45.4% of total cost saving relevant to the conventional design method. In addition, the results of the new water and energy minimization for example 2 showed 43.6% of fresh water, 60.3% of hot utility, 100% of cold utility, 70% of number of heat transfer units and 61.6% of total cost saving relevant to the conventional design method. Consequently, applying the presented methodology to the industrial large-scale problems can provide more water and energy conservational opportunities.

ACKNOWLEDGEMENTS

This work is supported by Brain Korea 21 project (environmental informatics program), the Korea Science and Engineering Foundation (KOSEF) grant funded by the Korea

NOMENCLATURE

A_{ij}	Inside tube surface area in separate system *j, m²*
A_{lmj}	Log mean of inside and outside tube surface areas in separate system *j, m²*
A_{oj}	Outside tube surface area in separate system *j, m²*
C	Cooler
C_{Aj}	Annual cost of heat exchanger per unit outside tube surface area in separate system *j, $/m²yr*
C_e	Annual cost of energy, *$/kWyr*
$C_{i,j,in}$	Average contaminant *j* concentration of inlet stream to operation *i, ppm*
C_{ij}	Cost of supplying 1 kW electricity to pump tube side fluid in separate system *j, $/kWyr*
$C_{i,j,out}$	Average contaminant *j* concentration of outlet stream from operation *i, ppm*
$C_{k,j,out}$	Average contaminant *j* concentration of outlet stream from operation *k, ppm*
C_{oj}	Cost of supplying 1 kW electricity to pump shell side fluid in separate system *j, $/kWyr*
C_w	Annual cost of fresh water, *$.h/t.yr*
$C^{\max}_{i,j,in}$	Maximum allowable concentrations of contaminant *j* at the inlet of operation *i, ppm*
D_{ij}	Tube inside diameter in separate system *j, m*
D_{oj}	Tube outside diameter in separate system *j, m*
E_{ij}	Power loss inside tubes per unit outside tube area in separate system *j, kW/m²*
E_{oj}	Power loss outside tubes per unit outside tube area in separate system *j, kW/m²*
f_{Aj}	A_{ij}/A_{oj}
f_i	Inlet fresh water flowrate to operation *i, t/h*
f_i^{fixed}	fixed flowrate of operation *i, t/h*
$f_{i,gain}$	increase in the flowrate through operation *i, t/h*
$f_{i,loss}$	water loss through operation *i, t/h*

C_p	Specific heat capacity, $kJ/kg^{o}C$
$C^{\max}_{i,j,out}$	maximum allowable concentrations of contaminant *j* at the outlet of operation *i*, *ppm*
$h_{f_i j}$	Fouling coefficient of inside tubes in separate system *j*, $W/m^{2o}C$
$h_{f_o j}$	Fouling coefficient of outside tubes in separate system *j*, $W/m^{2o}C$
h_{ij}	Coefficient of heat transfer inside tubes in separate system *j*, $W/m^{2o}C$
h_{oj}	Coefficient of heat transfer outside tubes in separate system *j*, $W/m^{2o}C$
h_{tj}	Combined coefficient for tube wall and dirt films in separate system *j*, $W/m^{2o}C$
k	Unit conversion factor, *0.2778*
k_{wj}	Thermal conductivity of tube wall in separate system *j*, $W/m^{o}C$
L_j	Lagrangian function for separate system *j*, $\$/yr$
L_{tj}	Length of tubes in separate system *j*, *m*
l'_j	Thickness of tube wall in separate system *j*, *m*
M_{ij}	Flowrate of fluid inside tubes in separate system *j*, *t/h*
Min	*Minimization*
N_{cj}	Number of clearances for flow between tubes across shell axis in separate system *j*
NLP	Non-linear programming
$n_{operations}$	Number of operations
N_{tj}	Number of tubes in the exchanger in separate system *j*
OPCOST	Total anuual cost of operating, $\$/yr$
$OP_{1,2,3,4}$	Water-using operations
Q_i	Energy requirement for heating of inlet freshwater stream to operation *i*, *kW*

F_{tj}	Multipass exchanger factor in separate system *j*
H	Heater
Q_{Recovery}	Heat recovery, *kW*
q_j	Rate of indirect heat transfer in separate system *j*, *kW*
S_{oj}	Minimum cross-sectional area for flow across tubes in separate system *j*, m^2
T	Temperature, ^{o}C
T_0	Temperature of freshwater source, ^{o}C
t_{1j}	Shell side inlet temperature in separate system *j*, ^{o}C
t_{2j}	Shell side outlet temperature in separate system *j*, ^{o}C
T_{1j}	Tube side outlet temperature in separate system *j*, ^{o}C
T_{2j}	Tube side inlet temperature in separate system *j*, ^{o}C
TC_j	Total annual cost of the heat exchanger in separate system *j*, $\$/yr$
T_{fi}	Temperature of inlet fresh water stream to operation *i*, ^{o}C
$T_{i,in}$	Average temperature of inlet stream to operation *i*, ^{o}C
$T_{i,out}$	Average temperature of outlet stream from operation *i*, ^{o}C
$T_{j,out}$	Average temperature of outlet stream from operation *j*, ^{o}C
U_{oj}	Overall coefficient of heat transfer based on outside tube area in separate system *j*, $W/m^{2o}C$
W_i	Flowrate of steam from operation *i* to wastewater treatment, *t/h*
$X_{i,k}$	Flowrate of stream from operation *k* to operation *i*, *t/h*
$X_{k,i}$	Flowrate of stream from operation *i* to operation *k*, *t/h*

Greek Letters

$\Delta m_{i,j,tot}$	Total mass transfer load of contaminant *j* in operation *i*, *kg/h*
$\Delta m^{fixed}_{i,j}$	change in concentration of contaminant *j* due to the fixed mass load of contaminant *j* transferred through operation *i*, *kg/h*
v_{ij}	Average velocity of fluid inside tubes in separate system *j*,*m/s*
v_{oj}	Average velocity of fluid outside tubes at shell axis in separate system *j*,*m/s*

ω_j	Lagrange multiplier for separate system *j*, $\$W/yr^{o}C$
φ_{ij}	Factor relating friction loss to h_{ij}
φ_{oj}	Factor relating friction loss to h_{oj}

government (MEST) (KRF-2009-0076129) and funded by Seoul R&BD Program (CS070160).

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