



Energy efficient water utilization systems in process plants

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Abstract

This paper introduces a new approach for the design of water utilization networks featuring minimum freshwater usage and minimum utility consumption in process plants. The procedure is confined to treat the single pollutant case, and it is based on a linear programming formulation that relies on necessary conditions of optimality and a heat transshipment model. An LP model is first solved to obtain minimum water usage and minimum heating utility target values. Once the energy and water targets have been identified, an MILP model is generated. This model, which accounts for non-isothermal mixing, provides the information needed to construct the water reuse structure as well as the corresponding heat exchanger network. © 2002 Elsevier Science Ltd. All rights reserved.

Keywords: Water utilization networks; Process plants; Energy minimization; Wastewater minimization

Nomenclature

c	cooling utility
C	cold process stream
C	concentration of contaminant (ppm)
CU_{\min}	minimum cooling utilities c
C_p	stream heat capacity, J/(kg °C)
D	set of cold streams that go from process p/r to process q/s
DE	set of cold streams that go from process k to wastewater collector u
DW	set of cold streams that go from fresh water source w to process j
F	water flowrate (kg/s)
H	hot process stream
HU_{\min}	set of heating utilities h
h	heating utility
Q	heat load (kW)
S	set of hot streams that go from process p/r to process q/s
SE	set of hot streams that go from process k to wastewater collector u
SW	set of hot streams that go from fresh water source w to process j
T	set of intervals t
T	water temperature (°C)
t	temperature interval
U	upper bound on the heat transfer (kW)
V	heat exchange between two streams (kW)

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Z	binary variable denoting the existence of a flowrate
ΔT_{\min}	minimum temperature approach ($^{\circ}\text{C}$)
α	minimum freshwater usage target (kg/s)
β	minimum heating utility target (kW)
δ	cascaded heat (kW)

Subscripts

$i, j, k, p, q,$ r, s, u	water-user process
in	at the inlet of a process
out	at the outlet of a process
P_j	precursor processes of process j
R_j	receiver processes of process j
t	temperature interval
w	fresh water

Superscripts

max	at the maximum
min	minimum
w	fresh water
*	additional sources

1. Introduction

Water and energy are among the most highly used commodities in industrial processes. Refineries and petrochemical plants spend water in big amounts for stripping, liquid–liquid extraction, and different washing operations. Large energy consumption in the form of heating and cooling utility is also required. After utilizing the water, these processes deliver wastewater, which may contain several contaminants. Therefore, wastewater treatment constitutes a primary concern in most industrial sites. Wastewater treatment has always focused on end-of-pipe solutions, which has been seen as the sole remedy to meet imposed discharge limits. Scarcity of water and stricter regulations on industrial effluents has created a different view on water usage. The possibility of selectively reusing wastewater within battery limits has become an option worth exploring. Wastewater reuse and/or recycle can be performed with or without intermediate treatment. This produces a direct impact in the overall amount of fresh makeup water usage as well as the amount of wastewater that reaches final treatment.

The concept of reusing water has received the name of water/wastewater allocation planning (WAP) problem. The search for optimal wastewater reuse solutions was addressed by industry itself more than 20 years ago (Carnes, Ford, & Brady, 1973; Skylov &

Stenzel, 1974; Hospondarec & Thompson, 1974; Mishra, Fan, & Erickson, 1975; Sane & Atkins, 1977). Later, two major systematic strategies were developed: the use of graphic targeting procedures coupled with heuristics, and the use of superstructures coupled with mathematical programming. Takama, Kuriyama, Shiroko, and Umeda (1977) used mathematical programming to solve a refinery example problem. A superstructure of all water using operations and cleanup processes was set up, and an optimization was then carried out to reduce the system structure by removing irrelevant and uneconomical connections. The authors transformed the model into a series of problems without inequality constraints by using a penalty function and finally solving it by using the complex method.

Wang and Smith (1994) presented a graphical method based on targeting, mostly useful for the single component case, with very limited extension to the multicomponent situation. The basic concept underlying the methodology is mass exchanger network (MEN) technology, which was in turn first proposed by El-Halwagi and Manousiouthakis (1989) and was applied to the removal of phenol from refinery wastewater (El-Halwagi & Manousiouthakis, 1990). In fact, the approach of Wang and Smith (1994) to determine optimal reuse solutions is in reality a special case of MENs. They also explored options of regenerating wastewater even when the pollutant level has

not reach the end-of-pipe conditions, or has not been reused throughout the entire process. The authors approached the WAP using targeting graphical representations and heuristic techniques for the design of the realizing network.

Kuo and Smith (1995) approached the WAP problem in combination with the wastewater clean-up allocation planning (WCAP) problem and use graphical representations and techniques on superstructures of alternative designs. Doyle and Smith (1997), and later Alva-Argáez, Kokossis, and Smith (1998), presented a solution approach for multicomponent systems based on mathematical programming. The problem is modeled as a nonconvex MINLP and then solved using a two-phase strategy. The authors of this paper stated that their approach does not guarantee optimality.

We now concentrate on further developments for the single component case. Savelski and Bagajewicz (2000) developed necessary conditions for the optimal water/wastewater allocation-planning problem. These conditions have been used together with some sufficient conditions of optimality to propose a method to build these networks by hand using simple calculations and rules (Savelski & Bagajewicz, 2001). Finally, the same authors proposed a linear programming formulation of the problem based on the aforementioned necessary conditions (Bagajewicz & Savelski, 2001). The WAP problem has been shown to have multiple solutions of the same cost. Finally, the influence of heat integration on the solution of the WAP problem has been ignored for a long time. Savelski and Bagajewicz (1997) first studied the problem pointing out the existence of a trade off. The design of an energy-efficient WAP was attempted by Savulescu and Smith (1998). They used a graphical procedure that does not seem suitable to be applied to all possible cases. Their method is sequential and will be revisited later in this paper and its limitations pointed out.

In this paper, a rigorous determination of the minimum freshwater usage and minimum utility consumption target values for water utilization networks is presented. Reduction of water consumption has been the typical objective function for this type of systems, as capital costs are not dominant. The reduction of utility consumption has been the first goal of most of the heat exchanger network design procedures. The procedure is based on the use of linear programming models. Once these targets are identified, an MILP model is built to obtain the corresponding heat exchanger network. The formulation allows the use of process-to-process connections as well as forbidden heat transfer matches. In addition, a method is proposed to obtain a merged-freshwater stream that exchanges heat with a merged-wastewater stream that is being sent to treatment.

2. Problem statement

Given is a set of water-using/water-disposing processes which required water of a certain quality and temperature. It is desired to determine a network of water-stream interconnections among the processes and to design a network of heat exchangers between these streams. The objective is the simultaneous minimization of the freshwater usage and the energy consumption of the whole system. Minimization of the water intake provides the processes with water of adequate quality, dictated by the given inlet and outlet concentrations limits, while minimization of the energy consumption efficiently integrates the heat exchanger network.

Several assumptions have already become standard in the literature. First, the level of contaminants is so low that the total flowrate can be considered constant. Second, the contaminant load is fixed and independent of the flowrate. Although this assumption can be challenged conceptually and even practically in some cases, it has been considered adequate for most of the systems analyzed. Finally, as it was discussed briefly in the introduction, the objective function is the simultaneous reduction of water intake and heating utility. This approach ignores capital costs, which for the case of water are reduced to piping (that are substantially lower than all the water treatment costs), and in the case of heat are governed/limited by the use of the minimum temperature approach. Thus, the assumption is that larger water intake will increase the heating utility, so the water intake is to be at the minimum regardless of other considerations. Moreover, the associated water network is assumed governed by the heat exchange opportunities. Another important assumption is that all the processes operate isothermally. That is, water and the process side fluid are at the same temperature before making contact. In practice it may happen that the process fluid heats or cools the water resulting in an exit temperature different from the inlet one. The effect of such generalization of the model is discussed in a separate section at the end of the paper.

3. Two-stage approach

Savulescu and Smith (1998) presented a method based on the following steps:

3.1. Stage 1

1. Obtain a water allocation network maximizing the energy transfer by mixing. The authors propose to use a two-dimensional grid diagram and the concept of water mains. This diagram allows them to identify heating and cooling duties graphically.

2. Apply certain re-use rules. These rules suggest starting the reuse structure from the hottest source, connect processes near in temperature, and use non-isothermal mixing.

3.2. Stage 2

1. Construct the energy composite curves and identify the minimum utility.
2. Assume all the freshwater is being sent to the processes as a single stream. Also, assume that the wastewater being sent to treatment is going to be merged appropriately.
3. Apply a set of splitting rules to obtain vertical matching of the composite curve portions.

The method is in reality a sequential procedure that makes use of certain heuristics in the first stage to obtain a network of process-to-process interconnections, such that the heat exchange structure might feature minimum utility. However, these rules cannot guarantee that the resulting structure is optimal. Moreover, the notion of connecting processes close in temperature may clash with the fact that monotonicity of outlet concentrations should hold (Savelski & Bagajewicz, 2000). In the illustration of the second stage, the authors assume that there are no process-to-process wastewater connections requiring heating or cooling in a heat exchanger. This

allows them to introduce the so-called separate systems. There are, however, processes where heating or cooling of the process-to-process streams is needed. The method of separate systems proposed does not address this case. Finally, to build the heat exchanger network, it is assumed that the wastewater streams are merged and sent to treatment. If one wants to send these streams to water treatment individually, at the least the concept of separate systems has to be re-formulated.

Savulescu and Smith (1998) proposed and solved an example that will be used in this paper to illustrate the features of our procedure. The data for this example are given in Table 1 and their proposed solution is illustrated in Fig. 1. The rest of the paper concentrates in introducing our procedure, which does not have the aforementioned limitations.

4. Necessary conditions of optimality

The following types of water-using processes have been introduced by Savelski and Bagajewicz (2000).

- Freshwater user processes (FWU): freshwater user processes are processes that require freshwater. They may also be consumers of wastewater.
- Wastewater user processes (WWU): wastewater user processes are processes that are fed solely by wastewater.

Table 1
Example data from Savulescu and Smith (1998)

Process number	Mass load of contaminant (g/s)	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 fresh water: $T_w = 20$ °C, temperature of wastewater: $T_{out} = 30$ °C.

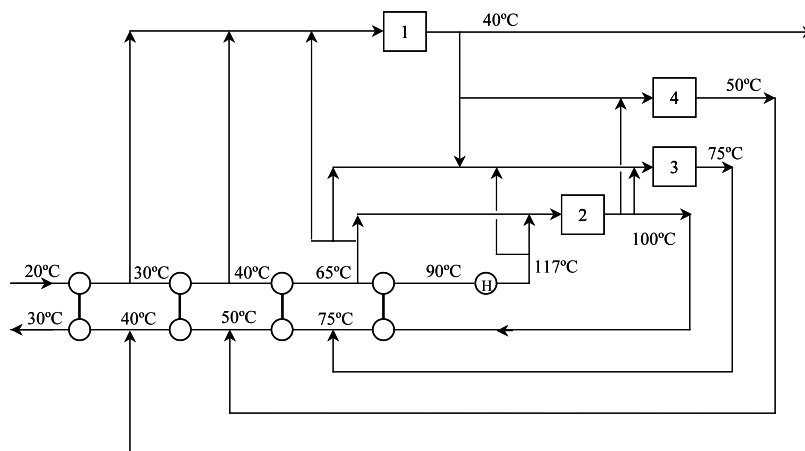


Fig. 1. Solution from Savulescu and Smith (1998).

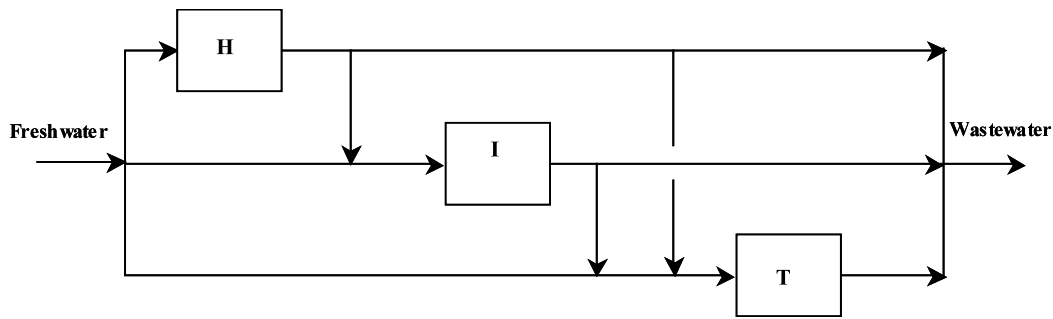


Fig. 2. Types of water using processes.

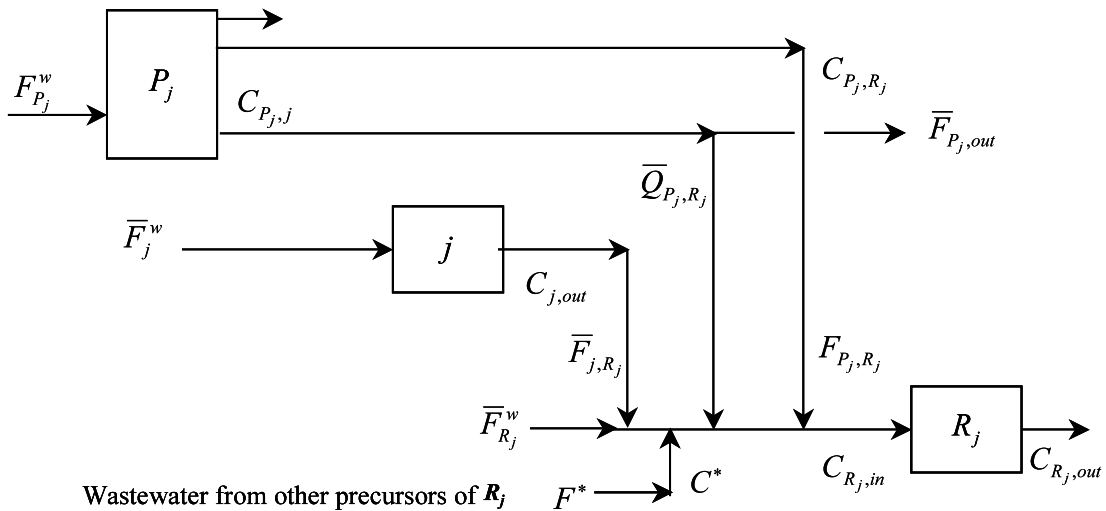


Fig. 3. Process interconnections of interest.

- Head processes (H): head process is a special case of a FWU that utilizes only freshwater.
- Intermediate wastewater user processes (I): intermediate wastewater user processes are processes that are fed by wastewater from other processes and feed other processes with the wastewater they produce.
- Terminal wastewater user processes (T): terminal wastewater user processes are processes that are fed by wastewater from other processes, but they discharge their wastewater to treatment.

Fig. 2 illustrates schematically the way these processes are aligned. The set of freshwater users consists of the set H and subsets of sets I and T. Similarly, the set of wastewater users is formed by a subset of I and a subset of T. That is, not all of the intermediate and terminal processes are using freshwater and/or are solely fed by wastewater.

The Following sets of water-using processes and additional types of processes were also introduced by Savelski and Bagajewicz (2000):

- Set of all processes (N): this set includes all water-using units.
- Set of head processes (H): This is the set of all head processes.

- Set of precursors of a process j (P_j): a set of precursors of a process is the set of all processes that send wastewater to process j .
- Set of receivers of process j (R_j): a set of receivers of a process is the set of all processes where wastewater from process j is sent.
- Partial wastewater providers (PWP): a partial wastewater provider is a process whose wastewater is partially reused by other processes. That is, a portion of its wastewater is sent directly to treatment.
- Total wastewater providers (TWP): a total wastewater provider is a process whose wastewater is fully reused by other processes.

Necessary conditions of optimality were introduced by Savelski and Bagajewicz (2000). These are briefly presented here for completeness, but the proofs are not repeated in this paper. Fig. 3 presents the set of interconnections of interest, omitting other existing ones that are not relevant to this case. The figure is taken from Savelski and Bagajewicz (2000) and is used in the proof of the theorem. Aside from the aforementioned precursor set P_j and the set of receivers R_j , the figure also shows the flow from the precursors to process j ($F_{P_j,j}$), the flow from process P_j to its receivers (F_{j,R_j}),

the flow from the precursors of process P_j directly to its receivers ($F_{P_j R_j}$), the fresh water feed to the precursors ($F_{P_j}^w$), process j (F_j^w) and the receivers ($F_{R_j}^w$), the flow from other processes (F^*) and the flow to treatment ($F_{j,out}$). Concentrations of pollutants for these streams are also indicated.

Theorem 1 (Necessary condition of concentration monotonicity). *If a solution to the WAP is optimal, then at every partial wastewater provider (PWP), the outlet concentrations are not lower than the concentration of the combined wastewater stream coming from all the precursors. In other words, given a process j that satisfies the definition of PWP, that is $F_{j,out} > 0$, then $C_{j,out} \geq C_{P_j}$, where C_{P_j} is the concentration of the combined wastewater of all the precursors.*

Theorem 2 (Necessary condition of maximum outlet concentration). *If a solution of the WAP problem is optimal, then all FWU processes have reached their maximum possible outlet concentration. Degenerate solutions with lower outlet concentrations may exist.*

These theorems are accompanied by a set of corollaries (Savelski & Bagajewicz, 2000), which are not essential for this paper.

5. Minimum fresh water targeting

The water allocation planning problem can be formulated as an NLP model (Bagajewicz & Savelski, 2001). We will assume that each water-using unit is characterized by a contaminant load L_j that needs to be entirely removed and by inlet and outlet maximum concentration constraints. The formulation of the NLP is as follows:

$$M1 = \text{Min} \sum_j F_j^w \quad (1)$$

s.t.

$$F_j^w + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,out} = 0 \quad \forall j \in N, i \in P_j, k \in R_j \quad (2)$$

$$F_h^w - \frac{L_h}{C_{h,out}^{\max}} = 0 \quad \forall h \in H \quad (3)$$

$$\left. \begin{aligned} \sum_i F_{i,j} (C_{i,out} - C_{j,in}) - F_j^w C_{j,in} &= 0 \\ \sum_i F_{i,j} (C_{i,out} - C_{j,out}) - F_j^w C_{j,out} + L_j &= 0 \end{aligned} \right\} \quad \forall j \in \bar{H}, i \in P_j \quad (4)$$

$$C_{j,in} \leq C_{j,in}^{\max} \quad \forall j \in \bar{H} \quad (5)$$

$$C_{i,out} \leq C_{i,out}^{\max} \quad \forall i \in P_j \quad (6)$$

Eq. (2) are water material balances around each process, while Eq. (3) are a pollutant balance in head processes. The first set of Eq. (4) represents the pollutant balances in the mixer before water is sent to each intermediate and terminal process, while the second set of equations represents the pollutant balances in those processes.

The problem has bilinear terms in those equality constraints where flowrate and concentration are simultaneously present. However, these bilinearities can be eliminated using the necessary condition of maximum outlet concentrations, that is, setting outlet concentrations to their maximum values. The constraints can now be combined as follows:

$$\left. \begin{aligned} \sum_i F_{i,j} (C_{i,out}^{\max} - C_{j,in}) - F_j^w C_{j,in} &= 0 \\ C_{j,in} &\leq C_{j,in}^{\max} \end{aligned} \right\} \Leftrightarrow \sum_i F_{i,j} (C_{i,out}^{\max} - C_{j,in}^{\max}) - F_j^w C_{j,in}^{\max} \leq 0 \quad \forall j \in \bar{H}, i \in P_j \quad (7)$$

$$\left. \begin{aligned} \sum_i F_{i,j} (C_{i,out} - C_{j,out}) - F_j^w C_{j,out} + L_j &= 0 \\ C_{i,out} &= C_{i,out}^{\max} \end{aligned} \right\} \Leftrightarrow \sum_i F_{i,j} (C_{i,out}^{\max} - C_{j,out}^{\max}) - F_j^w C_{j,out}^{\max} + L_j = 0 \quad \forall j \in \bar{H}, i \in P_j \quad (8)$$

The resulting problem is

$$M2 = \text{Min} \sum_j F_j^w \quad (9)$$

s.t.

$$F_j^w + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,out} = 0 \quad \forall j \in N, i \in P_j, k \in R_j \quad (10)$$

$$F_h^w - \frac{L_h}{C_{h,out}^{\max}} = 0 \quad \forall h \in H \quad (11)$$

$$\left. \begin{aligned} \sum_i F_{i,j} (C_{i,out}^{\max} - C_{j,in}^{\max}) - F_j^w C_{j,in}^{\max} &\leq 0 \\ \sum_i F_{i,j} (C_{i,out}^{\max} - C_{j,out}^{\max}) - F_j^w C_{j,out}^{\max} + L_j &= 0 \end{aligned} \right\} \quad \forall j \in \bar{H}, i \in P_j \quad (12)$$

This problem is linear. Consequently, the optimal water flowrate and a feasible realizing network are both obtained simultaneously. Furthermore, when setting up the problem, the number of variables can be reduced by not including non-monotone connections as suggested by the monotonicity necessary condition. Fig. 4 shows the water network obtained using M2 for the problem proposed by Savulescu and Smith (1998).

6. Minimum utility targeting

Bagajewicz and Savelski (2001) showed that problem M2 has several alternative solutions with the same water consumption. They exploited this property to find different networks featuring forbidden and compulsory matches, minimum number of interconnections, or minimum fixed cost. Furthermore, the degeneracy of this problem can be used to obtain the set of interconnections that feature minimum freshwater usage and minimum utility consumption simultaneously.

Once problem M2 is solved, a target for minimum freshwater usage is obtained. In order to obtain the minimum heating/cooling utility, this freshwater usage is to remain unchanged. Moreover, the water interconnections corresponding to this target can be ignored, as one is seeking a new set of interconnections, which features minimum-energy consumption while following the fixed freshwater target.

To build the model we consider the use of a Pinch Operator and a simplified version of the state-space representation of this problem, an approach proposed by Bagajewicz and Manousiouthakis (1992). This model was later used for heat exchanger networks and combined mass and heat exchange networks (Bagajewicz, Pham, & Manousiouthakis, 1998). Fig. 5 shows a state-space representation of the problem. A freshwater stream enters the distribution network where it is split and is sent to several junctions. These junctions also collect wastewater coming from processes (represented by the pollutant operator) and from heat exchangers (represented by a pinch operator). In turn, the pollutant operator has for this case the form of a superstructure operator (Bagajewicz et al., 1998), that is, each junction is connected to only one process. This is schematically shown in Fig. 6. Process streams transfer pollutants to the water.

Several models can be used to represent the pinch operator. Bagajewicz and Manousiouthakis (1992) proposed an MILP model that makes use of integers to take into account the varying position of the inlet and outlet temperatures and flowrates. In our case, however, inlet

and outlet temperatures can be considered fixed. This can be justified as follows. Assume that streams mix when they achieve their target temperature only. This means that the mixing junctions connected to the pinch operator receive a single stream coming from a process junction. This is illustrated in Fig. 7 and the corresponding flowsheet is shown in Fig. 8. Only one side of the heat exchangers is shown at each heating and cooling point.

The traditional version of the pinch operator considers classical heat transfer only and does not take into account the possibility of streams adjusting their temperatures through mixing. However, this mixing can be taken into account. Consider a hot and a cold stream (H_1 and C_1 , respectively). Fig. 9a shows the transshipment model cascade diagram obtained by the classical approach. In turn, Fig. 9b considers that H_1 and C_1 have been mixed. The remaining stream C'_1 is using the same amount of heating utility as in case a. Consequently, the assumption that mixing is taking place does not alter the result of the targeting problem. All this is possible because the hot and cold streams that mix have the same target temperature.

In view of the previous analysis, the state space representation of the process can be simplified eliminating splitting-to-mixing connections, maintaining the connections shown in Fig. 8 only. The pinch operator has now fixed inlet and outlet temperatures and varying flowrates. Fig. 10 shows the new situation.

The complete model to obtain the heating utility target is the following:

$$M3 = \text{Min} \left(\sum_{\forall h \in HU} Q_h \right) \quad (13)$$

s.t.

$$\sum_j F_j^w = \alpha \quad (14)$$

$$F_j^w + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,\text{out}} = 0 \quad \forall j \in N, i \in P_j, k \in R_j \quad (15)$$

$$F_h^w - \frac{L_h}{C_{h,\text{out}}^{\text{max}}} = 0 \quad \forall h \in H \quad (16)$$

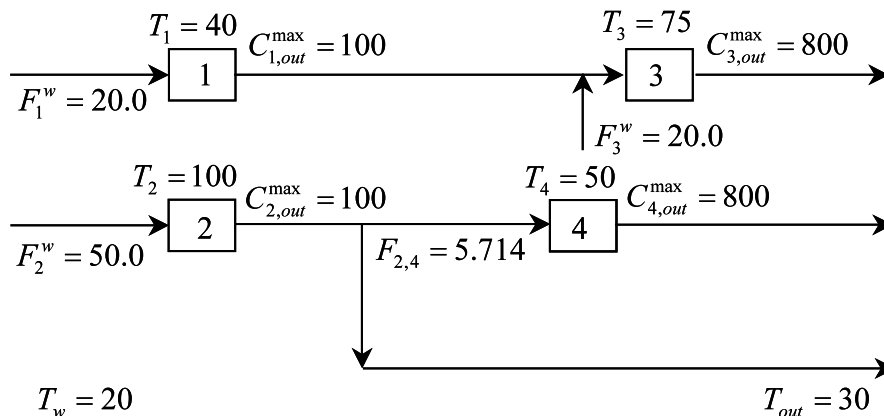


Fig. 4. Water network obtained using M2.

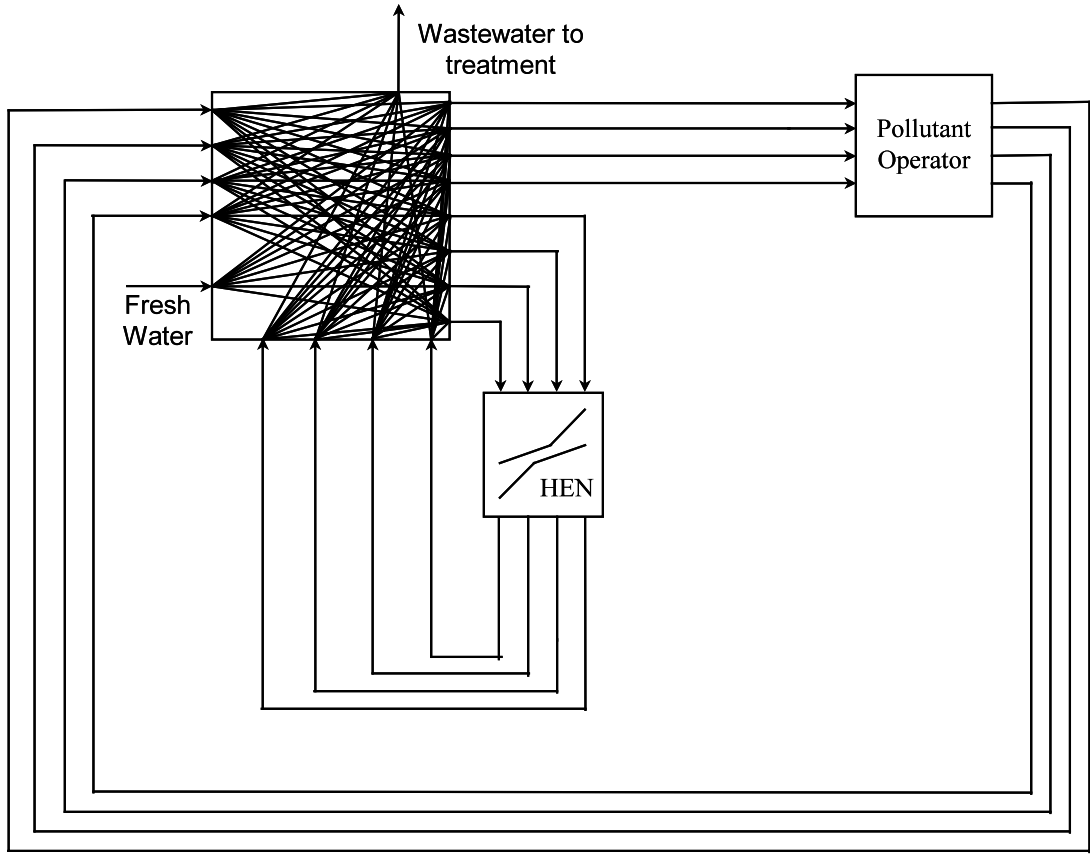


Fig. 5. State space representation.

$$\left. \begin{aligned} \sum_i F_{i,j} (C_{i,\text{out}}^{\max} - C_{j,\text{in}}^{\max}) - F_j^w C_{j,\text{in}}^{\max} &\leq 0 \\ \sum_i F_{i,j} (C_{i,\text{out}}^{\max} - C_{j,\text{out}}^{\max}) - F_j^w C_{j,\text{out}}^{\max} + L_j &= 0 \end{aligned} \right\} \quad \forall j \in \bar{H}, i \in P_j \quad (17)$$

$$\left. \begin{aligned} \delta_{h,t} - \delta_{h,(t-1)} + \sum_{(w,j) \in DW_t} V_{h,wj,t} + \sum_{(r,s) \in D_t} V_{h,rs,t} + \sum_{(k,u) \in DE_t} V_{h,ku,t} &= Q_h \quad t = t_h \\ \delta_{h,t} - \delta_{h,(t-1)} + \sum_{(w,j) \in DW_t} V_{h,wj,t} + \sum_{(r,s) \in D_t} V_{h,rs,t} + \sum_{(k,u) \in DE_t} V_{h,ku,t} &= 0 \quad t \geq t_h \end{aligned} \right\} \quad \forall h \in HU \quad (18)$$

$$\left. \begin{aligned} \delta_{wj,t} - \delta_{wj,(t-1)} + \sum_{(r,s) \in D_t} V_{wj,rs,t} + \sum_{(k,u) \in SE_t} V_{wj,ku,t} + \sum_{\forall c \in CU_t} V_{wj,c,t} &= F_j^w Cp_w (T_{t-1} - T_t) \\ \delta_{pq,t} - \delta_{pq,(t-1)} + \sum_{(w,j) \in DW_t} V_{pq,wj,t} + \sum_{(r,s) \in D_t} V_{pq,rs,t} + \sum_{(k,u) \in DE_t} V_{pq,ku,t} + \sum_{\forall c \in CU_t} V_{pq,c,t} &= F_{p,q} Cp_p (T_{t-1} - T_t) \\ \delta_{ku,t} - \delta_{ku,(t-1)} + \sum_{(w,j) \in SW_t} V_{ku,wj,t} + \sum_{(r,s) \in D_t} V_{ku,rs,t} + \sum_{\forall c \in CU_t} V_{ku,c,t} &= F_j^{\text{out}} Cp_k (T_{t-1} - T_t) \end{aligned} \right\} \quad \begin{aligned} &\forall (w,j) \in SW_t \\ &\forall (p,q) \in S_t \\ &\forall (k,u) \in SE_t \end{aligned} \quad \forall t \in T \quad (19)$$

$$\sum_{h \in HU_t} V_{h,wj,t} + \sum_{(p,q) \in S_t; q \neq j} V_{pq,wj,t} + \sum_{(k,u) \in SE_t} V_{ku,wj,t} \leq F_j^w Cp_w (T_{t-1} - T_t) \quad \forall (w,j) \in DW_t \quad \forall t \in T \quad (20)$$

$$\sum_{t \in N} \left(\sum_{h \in HU_t} V_{h,wj,t} + \sum_{(p,q) \in S_t} V_{pq,wj,t} + \sum_{(k,u) \in SE_t} V_{ku,wj,t} \right) = F_j^w Cp_w (T_C^t - T_C^s) \quad \forall (w,j) \in DW \quad (21)$$

$$\sum_{h \in HU_t} V_{h,rs,k} + \sum_{(w,j) \in SW_t; j \neq s} V_{wj,rs,t} + \sum_{(p,q) \in S_t; q \neq s} V_{pq,rs,t} + \sum_{(k,u) \in SE_t} V_{ku,rs,t} \leq F_{r,s} Cp_r (T_{t-1} - T_t) \quad \forall (r,s) \in D_t \quad \forall t \in T \quad (22)$$

$$\sum_{t \in N} \left(\sum_{h \in HU_t} V_{h,rs,k} + \sum_{(w,j) \in SW_t} V_{wj,rs,t} + \sum_{(p,q) \in S_t} V_{pq,rs,t} + \sum_{(k,u) \in SE_t} V_{ku,rs,t} \right) = F_{r,s} Cp_r (T_{t-1} - T_t) \quad \forall (r,s) \in D \quad (23)$$

$$\sum_{h \in HU_t} V_{h,ku,t} + \sum_{(w,j) \in SW_t} V_{wj,ku,t} + \sum_{(p,q) \in S_t} V_{pq,ku,t} = F_j^{out} Cp_j (T_{t-1} - T_t) \quad \forall (k,u) \in DE_t \quad \forall t \in T \quad (24)$$

$$\sum_{(w,j) \in SW_t} V_{wj,c,t} + \sum_{(p,q) \in S_t} V_{pq,c,t} + \sum_{(k,u) \in SE_t} V_{ku,c,t} = Q_c \quad \forall c \in CU_t \quad \forall t \in T \quad (25)$$

$$F_j^w, F_{i,j}, F_j^{out}, \delta, V, Q \geq 0$$

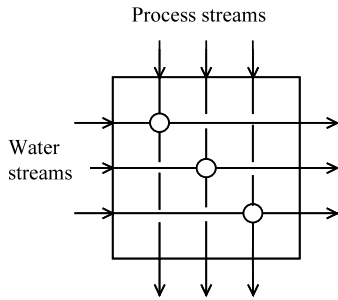


Fig. 6. Superstructure operator.

The model minimizes the heating utility and uses a fixed amount of freshwater, obtained by minimum water usage targeting. The proper degenerate set of water interconnections is found by the inclusion of the sets of constraints (Eqs. (15)–(17)). Finally, constraints (Eqs. (18)–(25)) consider the transshipment model representation of the Pinch operator.

7. Illustration

We continue illustrating the methodology using the

example the example from Savulescu and Smith (1998). We first note that the target temperatures for water entering each process of this problem are such that they can be achieved using mixing, that is, no heat exchange is needed. Fig. 11 shows the water network obtained solving the minimum utility targeting model M3 for this example. The required minimum heating utility is 3780 kW. Note that the water network differs from the solution obtained using the water allocation problem M2. Another important observation is that the utility targeting model produced an interconnection between processes 3 and 4 that has the same concentration as the outlet concentration of process 4. The connection (although feasible) contributes nothing to the water requirement of process 4. Thus, the connection contributes only to energy savings. However, this solution is not unique. To prove this, the connection between 3 and 4 was forbidden and the network shown of Fig. 4 was obtained, which has the same utility usage.

The heat-targeting model is useful in providing one of the feasible water networks that realizes the minimum heating utility. This minimum utility can also be predicted for certain cases in a more straightforward manner using the following equations:

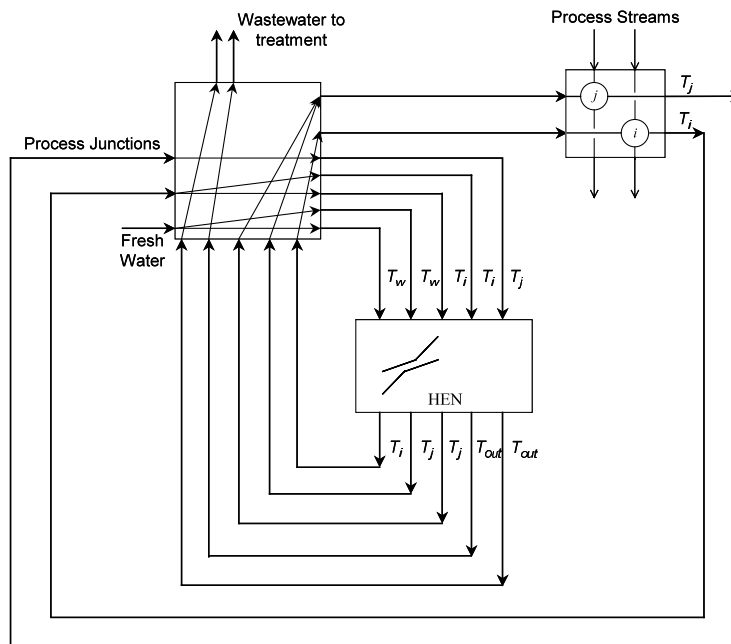


Fig. 7. Specific state space representation of the problem.

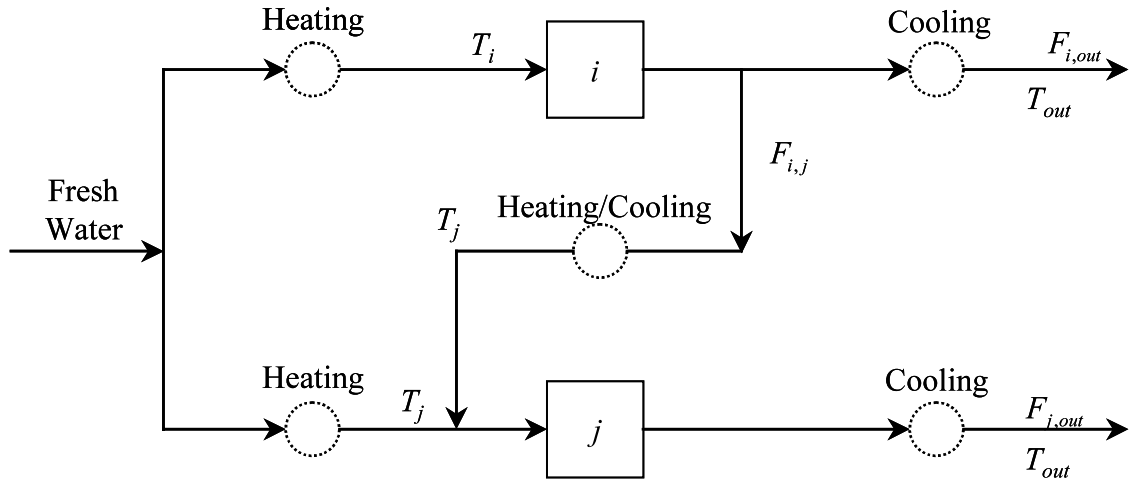


Fig. 8. Flowsheet corresponding to the state space representation.

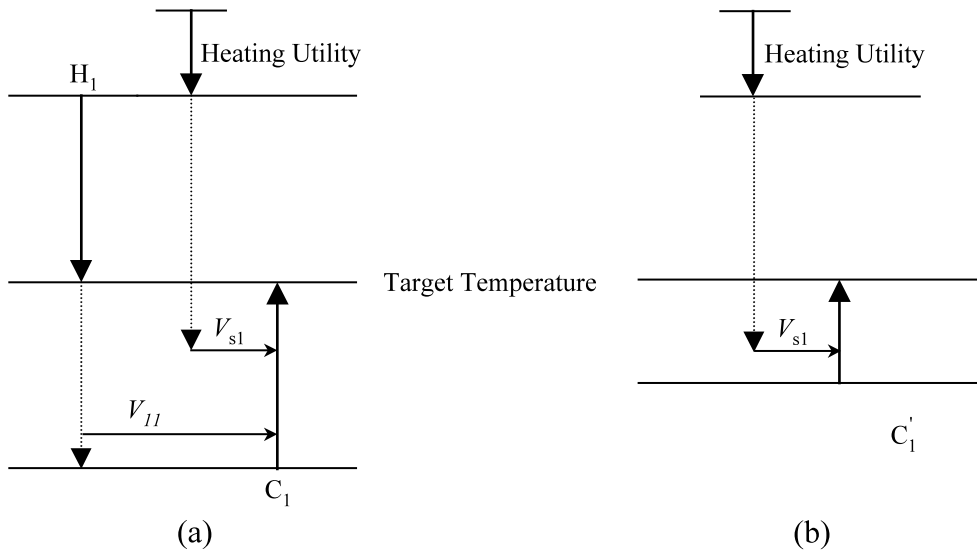


Fig. 9. Temperature adjustment of streams by mixing.

$$HU_{\min} = \alpha C_p \text{Max}\{T_{\text{out}} - T_{\text{in}}, \Delta T_{\min}\} \quad (26)$$

$$CU_{\min} = \alpha C_p \text{Max}\{\Delta T_{\min} - (T_{\text{out}} - T_{\text{in}}), 0\} \quad (27)$$

These equations are straightforward to understand in the context of a single process. However, in certain cases they also apply to the whole system. We explain this next and point out when they do not apply. Consider one process. The temperature vs. enthalpy diagram for this case is given in Fig. 12. Notice that two cases are immediately apparent.

1. $T_{\text{out}} - T_{\text{in}} \geq \Delta T_{\min}$: in this case, the problem is unpicked and the heating utility is given by Eq. (26). Fig. 12a illustrates this case.
2. $T_{\text{out}} - T_{\text{in}} < \Delta T_{\min}$: in this case, vertical alignment on the left is not possible (Fig. 12b). The heating

and cooling utilities are given by Eqs. (26) and (27), respectively.

For processes in which water undergoes continuous heating to a certain maximum temperature and this followed by cooling, the previous result holds. Indeed, consider the case where no heat transfer occurs through mixing. That is, water is always being heated up. This is shown in Fig. 13.

One can immediately recognize that mixing is another way of heat transfer, and therefore, covered by the above scenario. Thus, the following consideration follows: when all the wastewater has to reach the same outlet temperature, the heating and cooling utility is given by Eqs. (26) and (27).

In the example solved above, $F^w = 90.0$ kg/s, $C_p =$

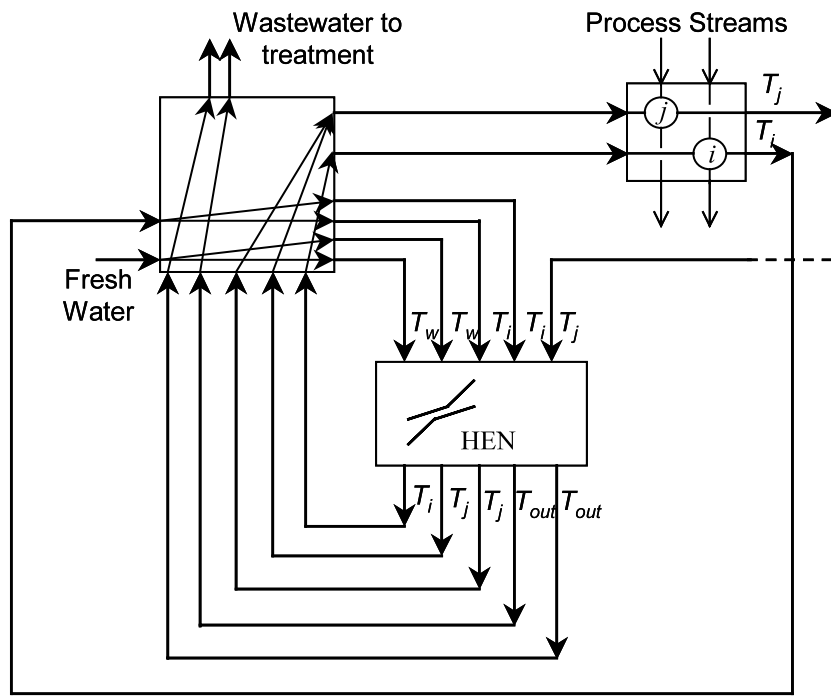


Fig. 10. State space simplification.

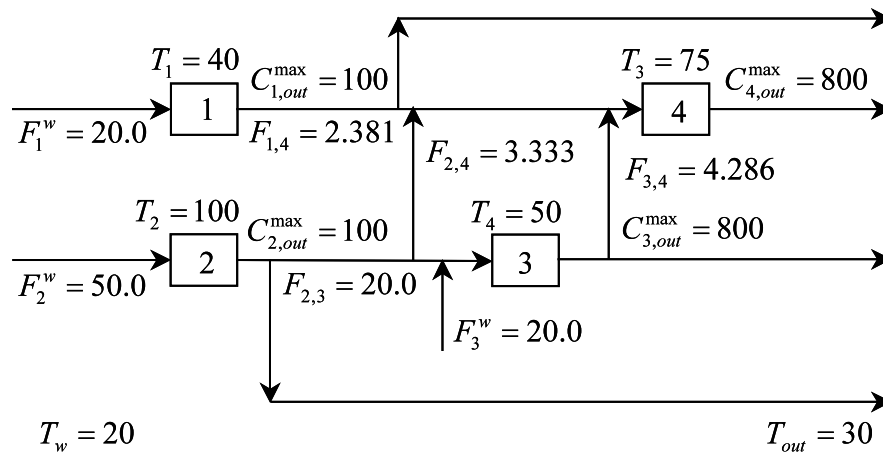


Fig. 11. Water network obtained using M3.

4.2 kW/kg °C and $T_{out}^w - T_{in}^w = 10$ °C, which gives 3780 kW. Any unrestricted feasible alternative solution of the water allocation problem M1 will in fact consume the same amount of utility regardless of the individual temperatures of the processes.

When water undergoes cycles of heating, followed by cooling at least one time, the above formulas may not hold. The formulas, however, provide a quick assessment of a lower bound on utilities. To illustrate this, consider the case of the problem given in Table 2. The solution is given in Fig. 14. The temperature versus

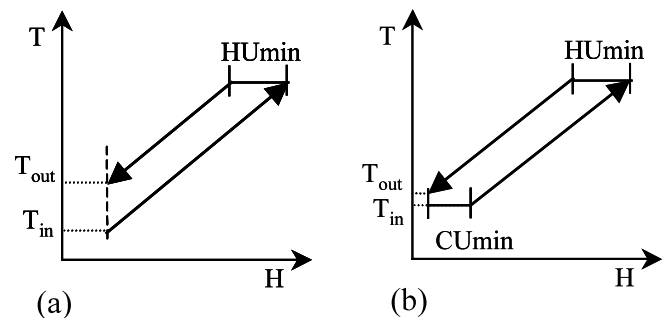


Fig. 12. Temperature vs. enthalpy diagram.

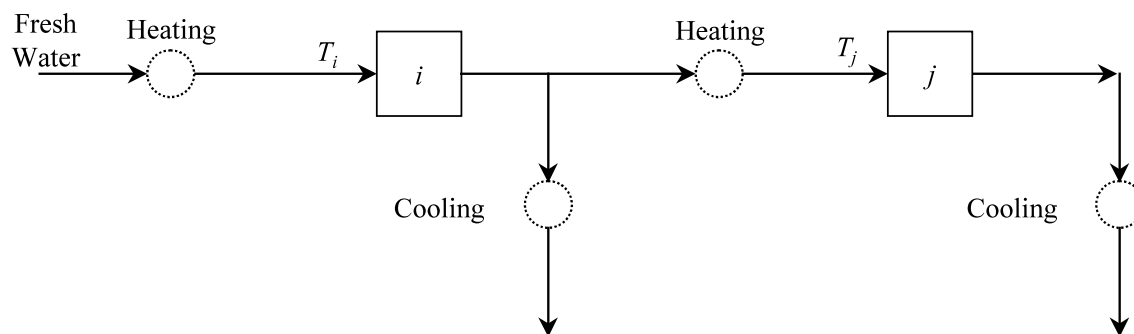


Fig. 13. Water heating followed by cooling.

Table 2
Illustrative example data

Process number	Mass load of contaminant (g/s)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature ($^{\circ}\text{C}$)
1	5	50	100	100
2	30	50	800	75
3	50	800	1100	100

Temperature of fresh water: $T_w = 20$ $^{\circ}\text{C}$, temperature of wastewater: $T_{out} = 30$ $^{\circ}\text{C}$.

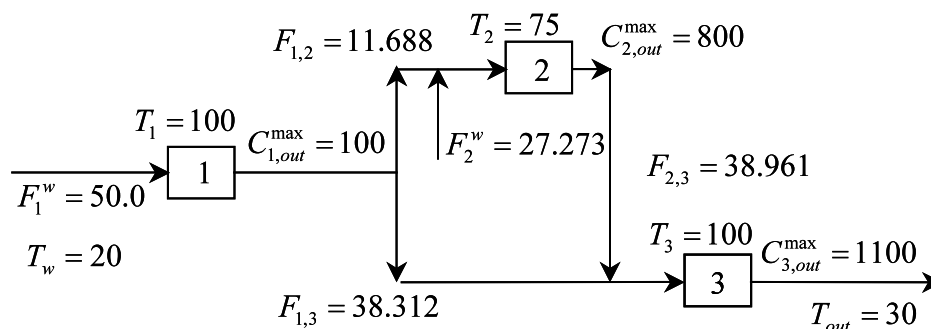


Fig. 14. Illustrative example solution.

enthalpy diagram is shown in Fig. 15, revealing that this is a pinched problem. Water from process 1 has to be used to heat up water going to process 3, and there is a limitation imposed by minimum temperature approach, which raises the minimum utility.

Moreover, the use of Eqs. (26) and (27) is not valid for the case in which one or more of the wastewater streams are sent to different treatment units and those units require different operating temperatures. This is illustrated using a modified version of the problem from Savulescu and Smith (1998). Consider the new temperature data given in Table 3.

This problem has the same fresh water target as the original formulation. However, the minimum heating

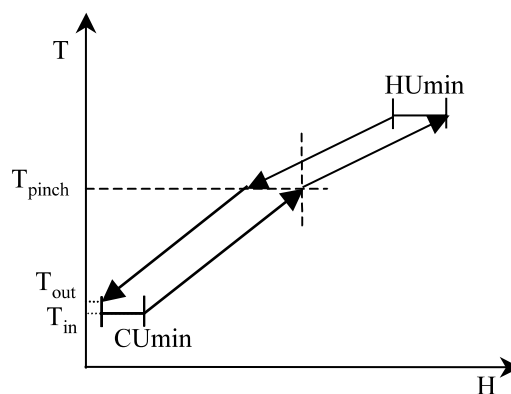


Fig. 15. Temperature vs. enthalpy diagram for the solution shown in Fig. 14.

Table 3
New temperature data for Savulescu and Smith (1998) example

Process number	Temperature (°C)	WWT temperature (°C)
1	40	30
2	100	60
3	75	40
4	50	30

Temperature of fresh water: $T_w = 20$ °C.

utility is now 8340 kW. Fig. 16 shows the resulting water network.

A compulsory water reuse between processes 1 and 3 is now imposed to be 15.238 ton/h with the intention of reproducing a water network structure similar to the one proposed by Savulescu and Smith (1998) (Fig. 1). Moreover, only heat exchange between wastewater and fresh-water is allowed. Fig. 17 shows the resulting water network. The heating utility of the corresponding heat exchanger network is 11,040 kW, which is larger than the optimum.

As one can see, if the water reuse network is obtained first, using ad-hoc considerations, one may obtain solutions that lead to larger utility consumption.

This example clearly shows that a two-stage approach in which target temperatures are forced by mixing can sometimes lead to a much larger heating utility than needed. Therefore, the problem needs to be solved considering the water and heating utility targets simultaneously.

8. Heat exchanger networks

Once the minimum utility target is obtained, a heat exchanger network can be constructed. If one uses the process-to-process flowrates and utility targets obtained from the previous steps, the problem reduces to a classical heat exchanger network design. However, one may decide to leave the constraints corresponding to the flowrate connections and build a generalized heat transshipment model. As this model is solved, new process-to-process connections and flowrates are chosen. In this way, the new structure is able to achieve a lower capital investment target. The problem can be written in compact form as follows:

$$M4 = \text{Min}\{\text{Number of Matches}\} \\ \text{s.t.}$$

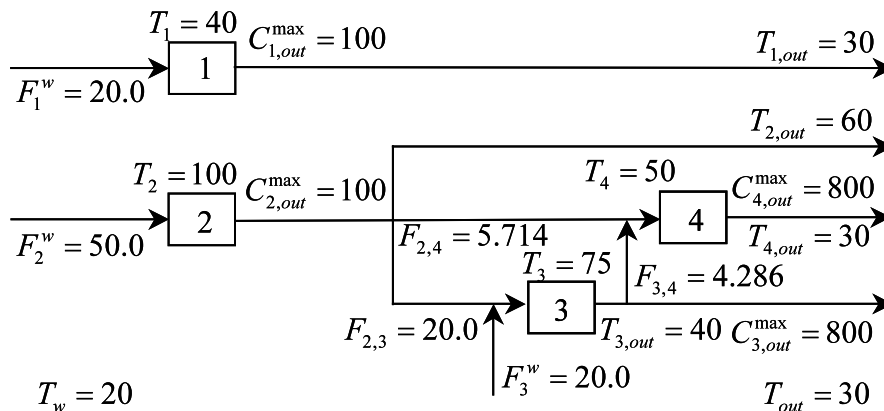


Fig. 16. Water network for Savulescu and Smith (1998) modified example.

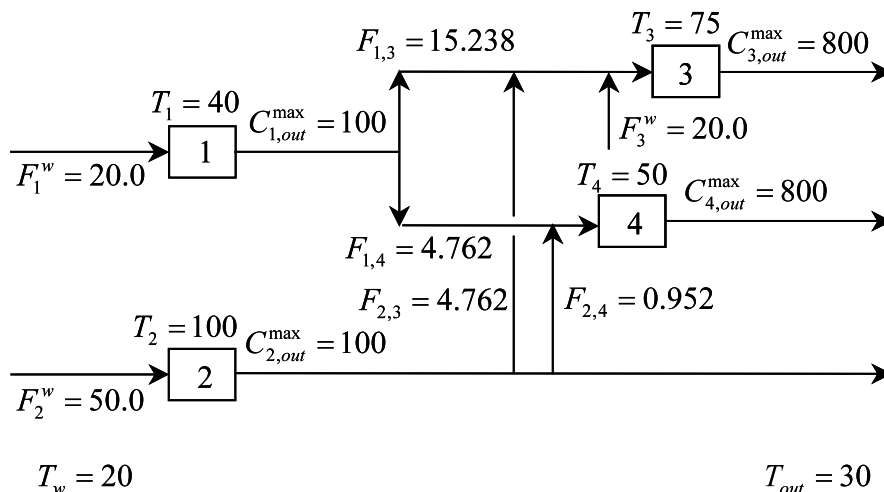


Fig. 17. Water network for compulsory water reuse.

Flowrate constraints

Heat balance constraints

Constraints counting matches

In this formulation, the objective function is given by:

$$\begin{aligned}
 \text{Min} = & \left(\sum_{\forall h \in HU; \forall (w,j) \in DW} Y_{h,wj} + \sum_{\forall h \in HU; \forall (r,s) \in D} Y_{h,rs} + \sum_{\forall h \in HU; \forall (k,u) \in DE} Y_{h,ku} + \sum_{\forall (w,j) \in SW; \forall (r,s) \in D; j \neq s} Y_{wj,rs} \right. \\
 & + \sum_{\forall (w,j) \in SW; \forall (k,u) \in DE} Y_{wj,ku} + \sum_{\forall (w,j) \in SW; \forall c \in CU} Y_{wj,c} + \sum_{\forall (p,q) \in S; \forall (w,j) \in D; q \neq j} Y_{pq,wj} + \sum_{\forall (p,q) \in S; \forall (r,s) \in D; q \neq s} Y_{pq,rs} \\
 & + \sum_{\forall (p,q) \in S; \forall (k,u) \in DE} Y_{pq,ku} + \sum_{\forall (p,q) \in S; \forall c \in CU} Y_{pq,c} + \sum_{\forall (k,u) \in SE; \forall (w,j) \in DW} Y_{ku,wj} + \sum_{\forall (k,u) \in SE; \forall (r,s) \in D} Y_{ku,rs} + \sum_{\forall (k,u) \in SE; \forall c \in CU} Y_{ku,c} \\
 & \left. + \sum_{\forall (k,u) \in SE; \forall (w,j) \in DW} Y_{ku,wj} + \sum_{\forall (k,u) \in SE; \forall (r,s) \in D} Y_{ku,rs} + \sum_{\forall (k,u) \in SE; \forall c \in CU} Y_{ku,c} \right) \quad (28)
 \end{aligned}$$

where the existence of a match between a pair of process streams or a stream and a heating or cooling utility stream is represented by the corresponding binary variable Y .

The flowrate constraints are given by Eqs. (13)–(17), and the heat balance constraints are given by Eqs. (18)–(25). The following target constraint is added.

$$\sum_{\forall h \in HU} Q_h = \beta \quad (29)$$

Finally, the following constraints used for counting heat matches are:

$$\left. \begin{aligned} \sum_{t \in N} V_{h,wj,t} - U_{h,wj} Y_{h,wj} &\leq 0 \quad \forall h \in HU; \quad \forall (w,j) \in DW \\ \sum_{t \in N} V_{h,rs,t} - U_{h,rs} Y_{h,rs} &\leq 0 \quad \forall h \in HU; \quad \forall (r,s) \in D \\ \sum_{t \in N} V_{h,ku,t} - U_{h,ku} Y_{h,ku} &\leq 0 \quad \forall h \in HU; \quad \forall (k,u) \in DE \end{aligned} \right\} \quad (30)$$

$$\left. \begin{aligned} \sum_{t \in N} V_{wj,rs,t} - U_{wj,rs} Y_{wj,rs} &\leq 0 \quad \forall (w,j) \in SW; \quad \forall (r,s) \in D; \quad j \neq s \\ \sum_{t \in N} V_{wj,ku,t} - U_{wj,ku} Y_{wj,ku} &\leq 0 \quad \forall (w,j) \in SW; \quad \forall (k,u) \in DE \\ \sum_{t \in N} V_{wj,c,t} - U_{wj,c} Y_{wj,c} &\leq 0 \quad \forall (w,j) \in SW; \quad \forall c \in CU \end{aligned} \right\} \quad (31)$$

$$\left. \begin{aligned} \sum_{t \in N} V_{pq,wj,t} - U_{pq,wj} Y_{pq,wj} &\leq 0 \quad \forall (p,q) \in S; \quad \forall (w,j) \in DW; \quad q \neq j \\ \sum_{t \in N} V_{pq,rs,t} - U_{pq,rs} Y_{pq,rs} &\leq 0 \quad \forall (p,q) \in S; \quad \forall (r,s) \in D; \quad q \neq s \\ \sum_{t \in N} V_{pq,ku,t} - U_{pq,ku} Y_{pq,ku} &\leq 0 \quad \forall (p,q) \in S; \quad \forall (k,u) \in DE \\ \sum_{t \in N} V_{pq,c,t} - U_{pq,c} Y_{pq,c} &\leq 0 \quad \forall (p,q) \in S; \quad \forall c \in CU \end{aligned} \right\} \quad (32)$$

$$\left. \begin{aligned} \sum_{t \in N} V_{ku,wj,t} - U_{ku,wj} Y_{ku,wj} &\leq 0 \quad \forall (k,u) \in SE; \quad \forall (w,j) \in DW \\ \sum_{t \in N} V_{ku,rs,t} - U_{ku,rs} Y_{ku,rs} &\leq 0 \quad \forall (k,u) \in SE; \quad \forall (r,s) \in D \\ \sum_{t \in N} V_{ku,c,t} - U_{ku,c} Y_{ku,c} &\leq 0 \quad \forall (k,u) \in SE; \quad \forall c \in CU \end{aligned} \right\} \quad (33)$$

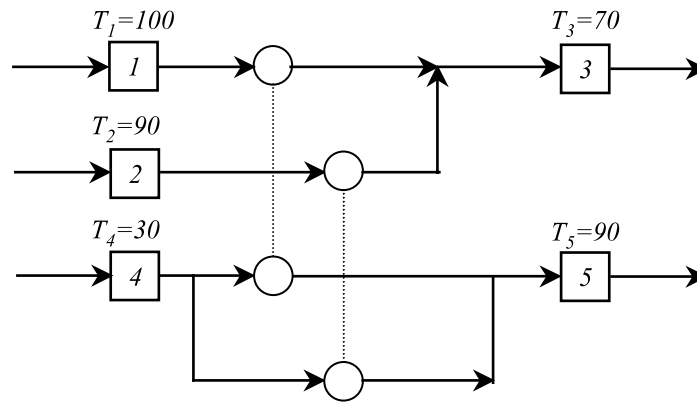


Fig. 18. Solution with two heat matches.

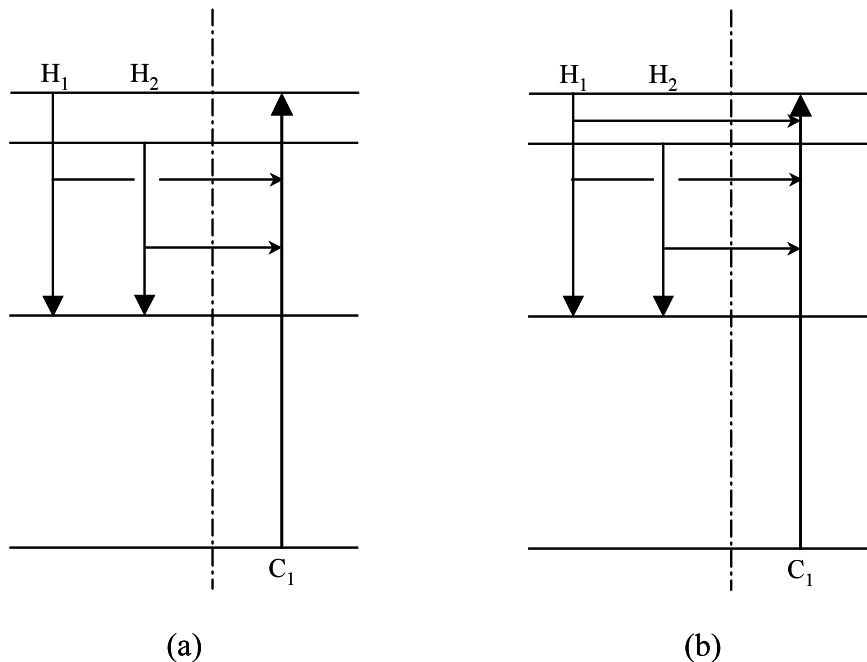


Fig. 19. Alternatives to the matches of Fig. 18.

$$F_j^w, F_{i,j}, F_j^{\text{out}}, \delta, V, Q \geq 0 \quad (34)$$

$$Y \in \{0, 1\} \quad (35)$$

Thus, the heat transshipment part of this model is again an extension of the model presented by Papoulias and Grossmann (1983) that considers variable flowrates. A few modifications have been introduced. First, the heat exchange between streams that are fed to the same process ($F_{i,j}$ and $F_{m,j}$) is not counted as a match. Therefore, the integer variables associated with a match between streams that can be mixed do not exist.

The above model may count heat exchangers twice. Consider the case of two streams going to the same process. Assume the solution obtained by the model shows that each of these streams matches exchanges

heat with the same cold stream. This situation is presented in Fig. 18, while Fig. 19 shows two alternative possibilities. In Fig. 19a, the hottest stream matches with the cold stream in the lowest interval. Therefore, one can assume that the two streams can merge before matching in a single heat exchanger. In Fig. 19b, the hottest stream realizes heat transfer in the highest interval, and even if merging of streams occurs, two heat exchangers are needed.

Fortunately, this situation if it is accounted by a revised model will not lead to a different solution, except in the matches between these three streams. The rest of the network is not altered by this. Therefore, instead of developing a new model, these situations can be identified after the solution is obtained and the merging can be performed.

9. Illustration

We now apply the heat transshipment model to the problem proposed by Savulescu and Smith (1998). If the heat exchange is omitted, the resulting water network is the one already shown in Fig. 17. The objective function value is 7. However, there is a pinch at 40 °C, which may explain why we were unable to find a network satisfying the minimum approach featuring 7 units. Nevertheless, a heat exchanger network featuring only 7 heat exchangers but with minimum approach violations and the same utility usage is possible (Fig. 20).

10. Merging of streams

The models previously presented do not consider the fact that the fresh water is coming from a unique source. Moreover, the freshwater to be sent to different processes can be progressively heated up in a set of exchangers, at the exit of which splitting to feed the processes can take place. The network already presented in Fig. 1 illustrates these observations. To achieve such a structure, the heat transshipment model was run allowing heat exchange between the fresh water inlet and wastewater streams only, that is forbidding process-to-process heat exchange. The water and heat

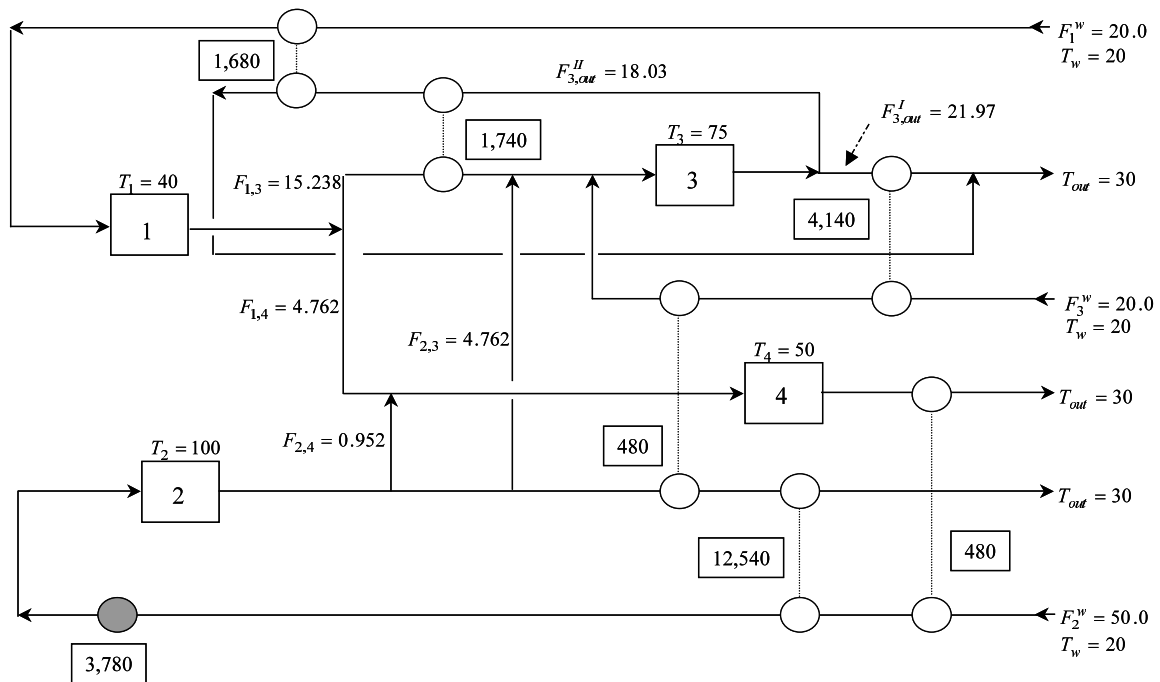


Fig. 20. HEN featuring minimum heating utility (example data from Savulescu & Smith, 1998).

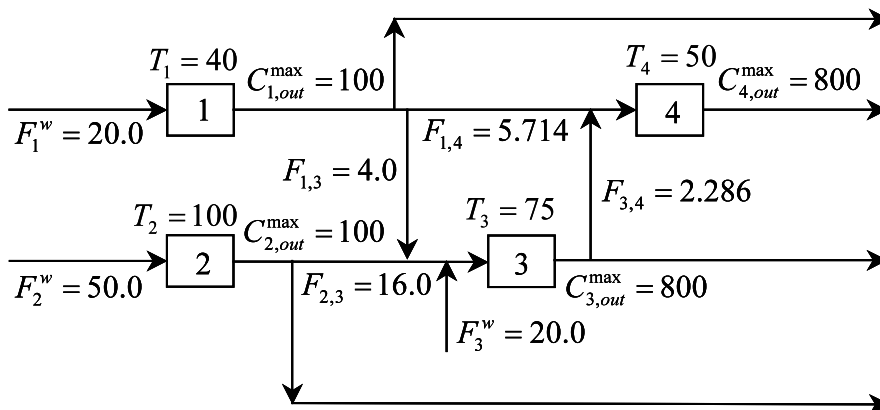


Fig. 21. Water network featuring minimum heating utility. Heat exchange in process-to-process streams forbidden.

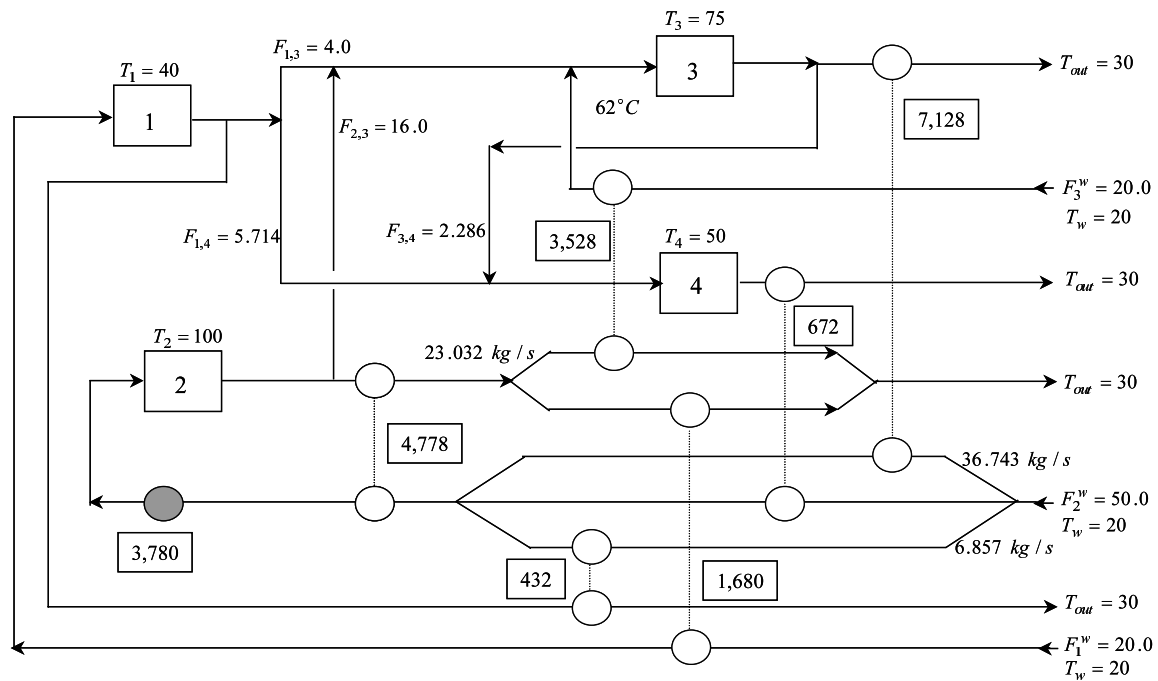


Fig. 22. HEN featuring minimum heating utility corresponding to the water network shown in Fig. 21.

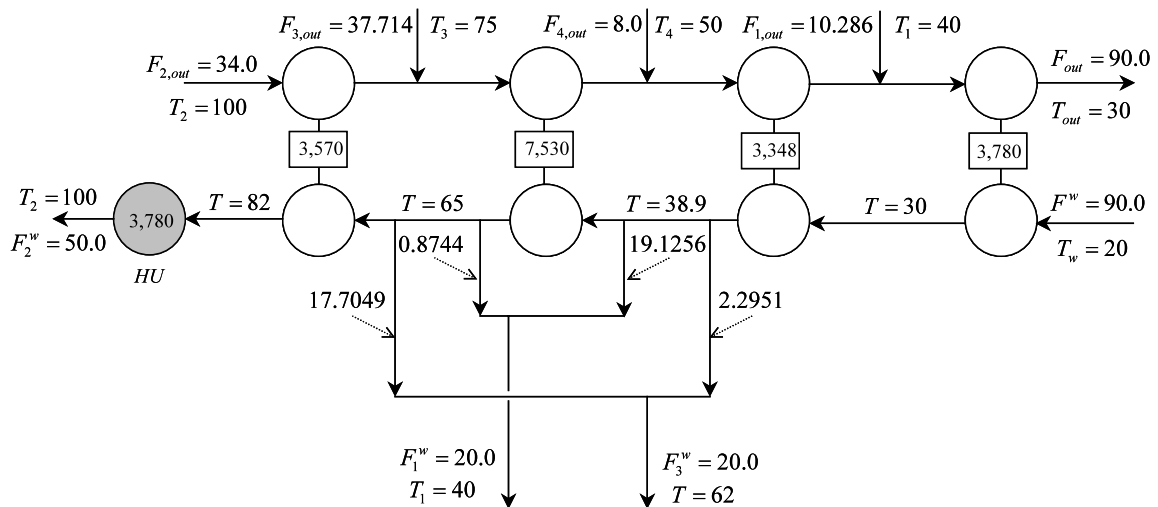


Fig. 23. Step 1 of the merging procedure.

exchanger networks are shown in Figs. 21 and 22, respectively. For the same reasons discussed in the case of the network of Fig. 20, the network of Fig. 22 features 7 units, has the same minimum utility usage but violates the minimum approach temperature.

Consider the network obtained following a merging procedure (Fig. 23). The total heat load exchanged by the streams has been redistributed among the temperature intervals in which it is exchanged. Consequently, a structure with only four heat exchangers and a heater is obtained.

Subsequent manipulations can be performed in this network to reduce the number of exchangers even further (Fig. 24).

Finally, an alternative solution with four heat exchangers is presented in Fig. 25. This network is a simplified version of the previous one since it features a single split in the outlet stream of process 3 instead of drawing fresh water at different temperatures and mixing them to provide processes 1 and 3. Therefore, the solution proposed requires fewer number of connections and is easier to control.

Remark 1. This merging procedure is not systematic and has been introduced to show that a structure of far less complexity than the one obtained by the two-step procedure suggested by Savulescu and Smith (1998) is possible. A transshipment model taking into account stream

mixing and splitting to achieve variable target temperatures is the appropriate answer to obtain these solutions automatically. Such a model will be presented in follow-up papers.

10.1. Compulsory and forbidden connections and matches

Forbidden connections and heat exchange matches can be obtained by simply setting the flowrate $F_{i,j}$ or the heat transferred $V_{i,j,k}$ to zero. For compulsory matches one could resort to the introduction of constraints of the type $F_{i,j} \geq F_{i,j}^{\min}$ and/or a similar one for heat transfer. However, this may lead to an infeasible

problem if such connection prevents the structure from achieving the targeted freshwater usage. This is the case when a connection between two processes that do not satisfy monotonicity is imposed. In such cases, one needs to go back to the fresh water-targeting model and solve it again including the desired compulsory connection.

An additional model can be constructed in which flows or heat loads in heat exchangers smaller than a certain threshold are forbidden. In other words, if the flow or the heat load exists, it should be higher than the threshold; otherwise is zero. This is accomplished by introducing the following constraints for flowrates.

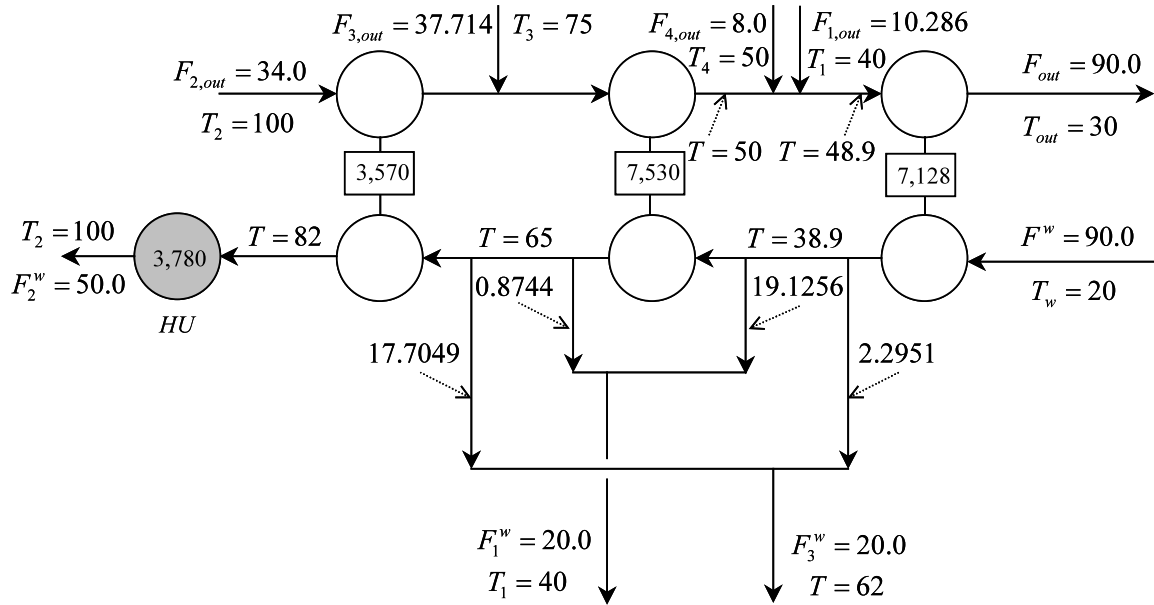


Fig. 24. Step 2 of the merging procedure.

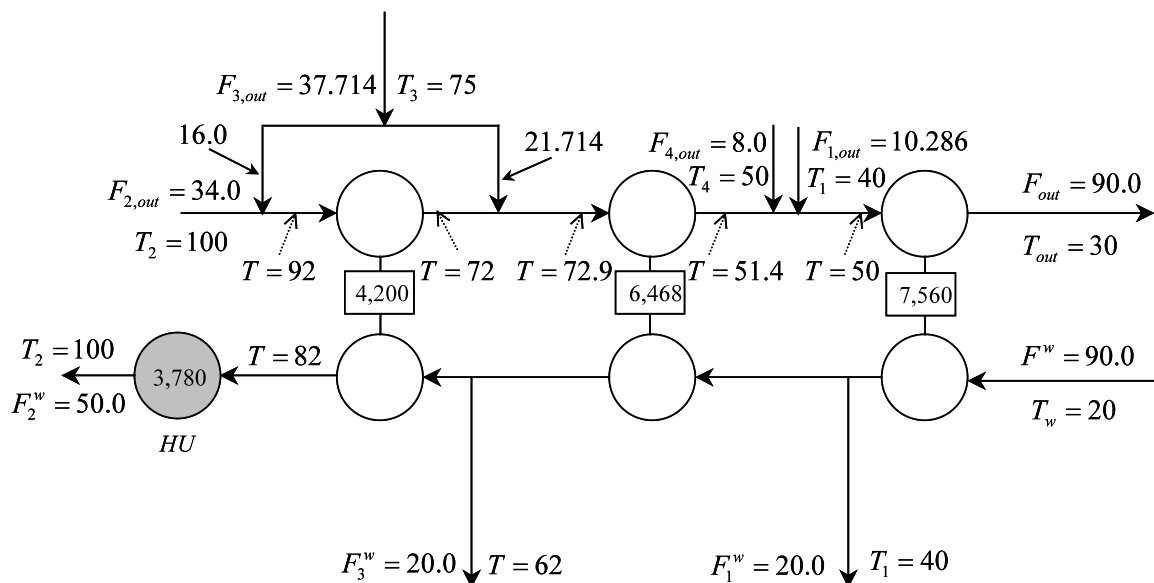


Fig. 25. Step 3 of the merging procedure.

Table 4
Data for the large system example

Process number	Mass load of contaminant (g/s)	C_{in}^{max} (ppm)	C_{out}^{max} (ppm)	Temperature (°C)
1	2.0	25	80	40
2	2.88	25	90	100
3	4.0	25	200	80
4	3.0	50	100	60
5	30.0	50	800	50
6	5.0	400	800	90
7	2.0	400	600	70
8	1.0	0	100	50

Temperature of fresh water: $T_w = 20$ °C, temperature of wastewater: $T_{out} = 30$ °C.

Table 5
Solution of the large system example

Process number	F (g/s)	C_{in} (ppm)	C_{out} (ppm)	Minimum fresh water flowrate with reuse (kg/s)
1	–	0	80	25.0
2	–	25	90	32.0
3	$F_{2,3} = 6.02$, $F_{4,3} = 0.29$	25	200	16.54
4	$F_{1,4} = 15.28$, $F_{2,4} = 19.75$	50	100	24.97
5	$F_{1,5} = 9.72$, $F_{2,5} = 6.22$, $F_{4,5} = 4.93$, $F_{8,5} = 1.69$	50	800	17.43
6	$F_{7,6} = 4.44$, $F_{8,6} = 5.87$	315.4	800	0.0
7	$F_{3,7} = 2.22$, $F_{4,7} = 2.22$	150	600	0.0
8	–	0	100	10.0

Total minimum fresh water flowrate (g/s) = 125.94.

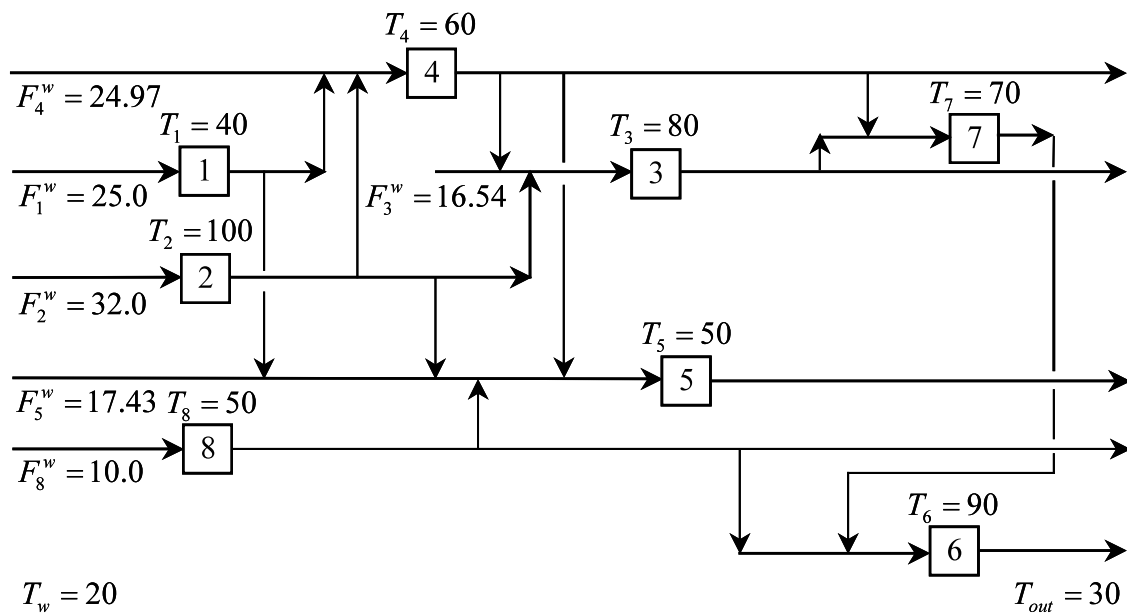


Fig. 26. Water network for the problem of Table 4.

$$\left. \begin{aligned} F_{i,j} &\leq F_{i,j}^* Z_{i,j} \\ F_{i,j} - U_{i,j} Z_{i,j} &\leq 0 \end{aligned} \right\} \quad (36)$$

Similar constraints can be written for heat loads in terms of $Y_{i,j}$ and $V_{i,j,k}$.

10.2. Illustration of the method for a large system

Consider a system of eight processes and its data that are presented in Table 4.

Table 5 shows all the resulting flowrates and final

concentrations of the processes, while Figs. 26 and 27 show the water network and the heat exchanger network, respectively. The heating utility and number of matches obtained are 5289.6 kW and 12, respectively.

11. Limitations

We now return briefly to discuss the issue of the temperature at the processes. The model presented considers the whole process as isothermal. In other words, the process streams are heated or cooled down to the desired temperature before being put in contact with water at the same temperature. This simplification allows the treatment of the problem as two separate ones, the design of the water network first and heat recovery later, effectively obtaining two independent and sequential problems. If one allows heat transfer between process streams and water, then the heat integration on the process side and on the water system become mutually dependent. In other words, the transshipment model used in this paper needs to be augmented to include the constraints for the process-to-process heat integration. While such an approach makes sense in principle, it requires the simultaneous design of both systems, something that rarely takes place in practice nowadays, but may happen in the future. Nevertheless, some simplifications can be performed to decouple the problems. This is future work.

Another important limitation of the present approach is that it does not address water networks with multiple contaminants. While mathematical programming models can be constructed (Doyle & Smith, 1997; Alva-Argáez, Kokossis, & Smith, 1998), these models are non-linear and difficult to solve. At the same time they cannot guarantee global optimality. Recent work along the line of making advantage of necessary conditions has been performed, leading to a method that can guarantee global optimality and does not have convergence difficulties (Savelski, Rivas, & Bagajewicz, 1999). Future work will exploit this problem representation and will attempt to incorporate the issue of heat to the design of systems with multiple contaminants.

12. Conclusions

A new method for obtaining energy-efficient solutions to the water allocation problem in refineries and process plants has been presented. The method relies on two sequential LP problems to obtain the freshwater usage and energy consumption targets. An MILP transshipment model formulation allows the building of the corresponding heat exchanger network. Finally, a merging procedure has been proposed to obtain structures where freshwater is delivered to the corresponding processes, as a split from a main freshwater stream that is

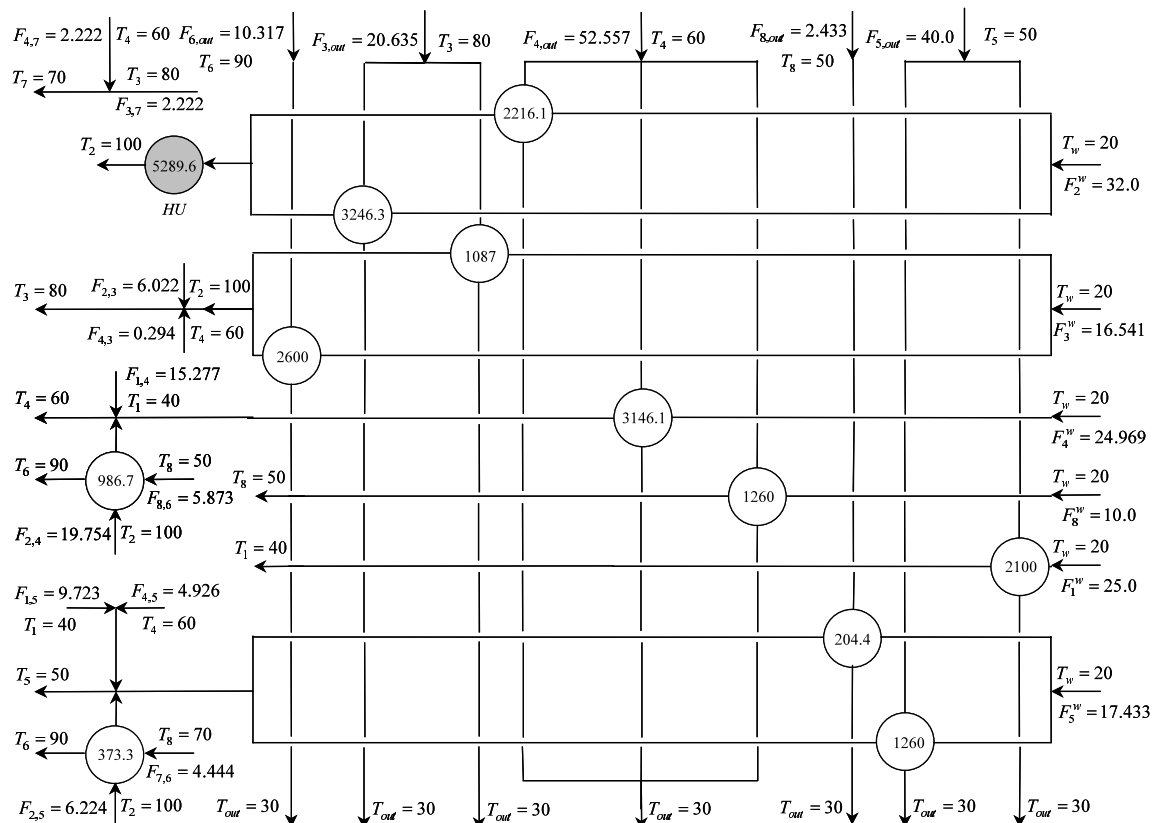


Fig. 27. Heat exchanger network for the problem of Table 4.

being heated up. A model to perform this step automatically using mathematical programming is the object of future work. The proposed methodology has been shown to take into account the interaction between water allocation and heat minimization simultaneously and with global optimality, proving that it can be superior to the two-step procedure proposed by Savulescu and Smith (1998), which cannot even guarantee local optimality. In addition, the procedure developed can incorporate forbidden and compulsory flow connections and heat transfer matches, an issue that is very important in the design of these systems as the processes can be geographically distant.

Acknowledgements

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