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Synthesis of non-isothermal heat integrated water networks in chemical processes

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ABSTRACT

This paper presents a new approach for the simultaneous synthesis and optimization of heat integrated water networks. A new superstructure for heat exchanger network (HEN) synthesis is proposed. The procedure is based on mixed integer non-linear mathematical programming (MINLP). Four relevant examples are presented to illustrate various aspects of the proposed approach.

1. Introduction

Water and energy are among the most important commodities used in the process industries. For example, water is used in petrochemical plants and refineries for stripping and liquid–liquid extraction; in iron and steel industries primarily as a coolant, in food and agricultural industries in a variety of washing operations. In certain situations significant amounts of water need to be heated up or cooled down to meet process operating conditions. As a consequence, large energy consumption in the form of cooling and heating utilities is needed. In such cases, when both the quality and temperature of water are important, water and energy management need to be considered simultaneously.

Different methods, rooted in conceptual design or mathematical programming, have been developed for water minimization as well as for the heat exchanger network (HEN) synthesis problem. The reader is referred to Bagajewicz (2000) for a comprehensive review of technologies developed to solve the water minimization problem and to Furman and Sahinidis (2002) for a review of the HEN synthesis technologies.

The most widely used technology in HEN synthesis field is the well-known Pinch Technology (Linnhoff, Townsend, Boland, & Hewitt, 1982). However, designs using the pinch methodology were shown to be in many cases non-optimal, mainly due to its sequential nature (minimize energy first, followed by strict unit number minimization), although some improvements have been noted (Supertargeting). To overcome the drawbacks of the pinch method different approaches using mathematical programming were presented over the last two decades. Of these, one can classify them as transportation–transshipment oriented and superstructure oriented. One of the latest models on the transportation–transshipment type is the one proposed by Barbaro and Bagajewicz (2005), which is linear and allows non-isothermal mixing as well as multiple matches between two streams. Among the superstructure-based models, the most popular method is a stage-wise superstructure approach (Yee & Grossmann, 1990).

Simplicity of pinch methodology and some similarities between water minimization and energy minimization problem induced a development of conceptual design approaches in the field of water minimization (Majozi, Brouckaert, & Buckley, 2006; Wang & Smith, 1994). The conceptual approach is mostly useful for the single-contaminant case, with very limited applicability to multi-contaminant cases. Multiple contaminant water problems require more elaborate methods (Karuppiah & Grossmann, 2006; Savelski, Rivas, & Bagajewicz, 1999).

Despite all the enabling technologies the influence of heat integration on the solution of water allocation planning (WAP) has been scarcely addressed in past years. Savelski and Bagajewicz (1997) first studied the problem pointing out the existence of a trade off. A

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Nomenclature

Indices

i	hot process stream
j	cold process stream
k	temperature location and stage index
l	contaminant
mx	mixer unit
n, m, fw, ww	stream
p	process unit
r	regeneration unit
s	splitter unit

Sets

CP	cold process streams
HP	hot process streams
M	mixer units
P	process units
R	regeneration unit
S	splitter units
ST	stages

Parameters

$c^{l}_{\mathrm{IN}_{\max}p}$, $c^{l}_{\mathrm{OUT}_{\max}p}$	maximal inlet/outlet concentration of contaminant l for process p (mg/kg)
C_{HE}	fixed costs for heat exchangers ($)
C_{A}	area cost coefficients ($/m^2)
C_{CON}	fixed costs for HEN connections ($)
C_{HU}	hot utility costs ($/(kW a))
C_{CU}	cold utility costs ($/(kW a))
C_{FW}	fresh water costs ($/t)
C_{R}	costs of waste water regeneration ($/t)
$C_{\mathrm{R,v}}$	regeneration unit capacity cost ($ h/t)
Cp	heat capacity (kJ/kg K)
EMAT	exchanger minimum approach temperature
$f_{\mathrm{a}}/1$	time fraction of operation
h	stream heat transfer coefficient (kW/(m^2 K))
L^{l}_{p}	mass load of contaminant l in process p (kg/s)
N_h	number of hours per year (h/a)
NOK	number of stages
T^{FWS}	temperature of fresh water source (K)
T^{WWS}	temperature of waste water sink (K)
U	overall heat transfer coefficient (kW/(m^2 K))
Γ	upper bound for temperature difference (K)
Ω	upper bound for heat exchange (kW)
$\alpha/1$	exponent for regeneration unit capacity
$\beta^{l}/1$	exponent for area cost
$\eta^{l}/1$	removal efficiency

Continuous variables

$CF^{\mathrm{H,IN}}_{i}$, $CF^{\mathrm{C,IN}}_{j}$	inlet heat capacity flow rate of hot stream i, and cold stream j (kW/K)
$CF^{\mathrm{H}}_{i,k}, CF^{\mathrm{H}'}_{i,i,k}, CF^{\mathrm{H}'}_{i,k}$; $CF^{\mathrm{C}}_{j,k}, CF^{\mathrm{C}'}_{j,j,k}, CF^{\mathrm{C}'}_{j,k}$	heat capacity flow rate of hot (kW/K) stream i, and cold stream j
F	mass flow rate (kg/s)
T^{IN}_{i}, T^{IN}_{j}	inlet temperature of hot stream i, and cold stream j (K)
$T_i, T'_{i,k}$; $T_j, T'_{j,k}$	temperature of hot stream i, and cold stream j (K)
$\Delta T_{\mathrm{H}\,i,j,k}$	temperature approach for match (i,j) in hot end of stage k (K)
$\Delta T_{\mathrm{C}\,i,j,k}$	temperature approach for match (i,j) in cold end of stage k (K)
$\Delta T_{\mathrm{CU}\,i}$	temperature approach for match of cold utility and hot stream i (K)
$\Delta T_{\mathrm{HU}\,j}$	temperature approach for match of hot utility and cold stream j (K)
$q_{i,j,k}$	heat exchanged between streams i and j in stage k
$q_{\mathrm{CU}\,j}$	heat exchanged between hot stream i and cold utility (kW)
$q_{\mathrm{HU}\,j}$	heat exchanged between cold stream j and hot utility (kW)

Binary variables

$z_{i,j,k}$	existence of heat exchanger for match (i,j) in stage k
$Z_{\mathrm{CU}\,i}$	existence of heat exchanger for match (cold utility, i)
$Z_{\mathrm{HU}\,j}$	existence of heat exchanger for match (hot utility, j)
$y^{\mathrm{H}}_{i,i,k}, y^{\mathrm{C}}_{j,j,k}$	existence of splits of hot and cold streams in HEN

Subscripts/superscripts

CU	cold utility
FW	fresh water
FWS	fresh water source
HU	hot utility
HEN	heat exchanger network
IN	inlet
LO	lower
OUT	outlet
UP	upper
WW	waste water
WWS	waste water sink
WN	water network

graphical procedure was introduced by Savulescu and Smith (1998) attempting to solve the energy efficient WAP problem. The method they used is sequential and was recently extended to consider water and heat minimization simultaneously (Savulescu, Kim, & Smith, 2005a; Savulescu, Kim, & Smith, 2005b). However, the approach is limited to a single-contaminant case. In turn, Bagajewicz, Rodera, & Savelski (2002) solved the problem using mathematical programming. With minor modifications their approach can be extended to handle the multi-contaminant case. The model is, nonetheless, sequential.

An important realization about all these systems is that, in the absence of regeneration, systems are pinched at the lowest (inlet) temperature. In addition, what makes the design challenging is that mixing of streams is a part of the design, especially if mixing of streams is used to achieve target temperatures, and therefore avoid the use of heat exchangers or utilities. It has been shown that clever mixing can reduce the number of exchangers in the system (Bagajewicz et al., 2002; Savulescu, Sorin, & Simth, 2002).

This paper introduces a new approach for simultaneous synthesis of energy efficient water networks, portions of which have been advanced, without the inclusion of important details, by Bogataj and Bagajewicz (2007). The model is MINLP and the main feature of the formulation is mixing and splitting of streams within the HEN superstructure, thus enabling direct heat exchange in order to reduce the number of heat exchangers as well as to reduce the complexity of heat integrated process structure.

2. Problem statement

Given is a set of water using/water disposing processes, which require water of adequate quality and temperature. The objective is to determine the optimal network of water stream interconnections among the processes and the corresponding heat exchanger network by simultaneously optimizing annual operating costs (fresh water, regeneration, and utility costs), and capital costs (heat exchanger costs). The following assumptions are used:

- The level of contaminant is low enough that the total flow rate can be considered constant,
- processes operate isothermally or non-isothermally (fixed temperature change),
- water is present only in a liquid phase,
- fresh water is free of contaminants,
- streams have constant heat capacity ($Cp = 4.186$ kJ/(kg K)),
- heat transfer coefficients are constant,
- heat exchangers are countercurrent,
- only one hot and one cold utility are available,
- no heat losses are considered for process streams.

3. Superstructure

In this section three superstructures relevant to this work are presented. Firstly, a simple superstructure for the synthesis of water networks, similar to the one presented by Alva-Argáez, Kokossis, and Smith (1998), is depicted in Fig. 1a. A set of water using process units (P) is interconnected using a set of mixer units (M) and a set of splitter units (S). A single regeneration unit (R), if embedded in the WN superstructure (Fig. 1b), accepts contaminated water from all the water using process units, selectively removes contaminants, and distributes treated water back to the water using process units. No self-recycling was considered in this work. Dashed lines are the only ones allowed to exchange heat in heat exchangers. We discuss this choice in detail later.

For the heat exchange, the stage-wise superstructure (Yee & Grossmann, 1990) for HEN synthesis was modified to account for direct heat exchange (mixing of streams) as well as the regular heat exchangers for indirect heat transfer. Fig. 2 presents a 2-hot–2-cold streams representation of the modified stage-wise superstructure. In this superstructure, each hot/cold stream can potentially mix with other hot/cold streams in each stage of the superstructure. We omit the detailed description of the basic features of the original model because they are well-known and concentrate on the additions: the mixing of streams at each stage.

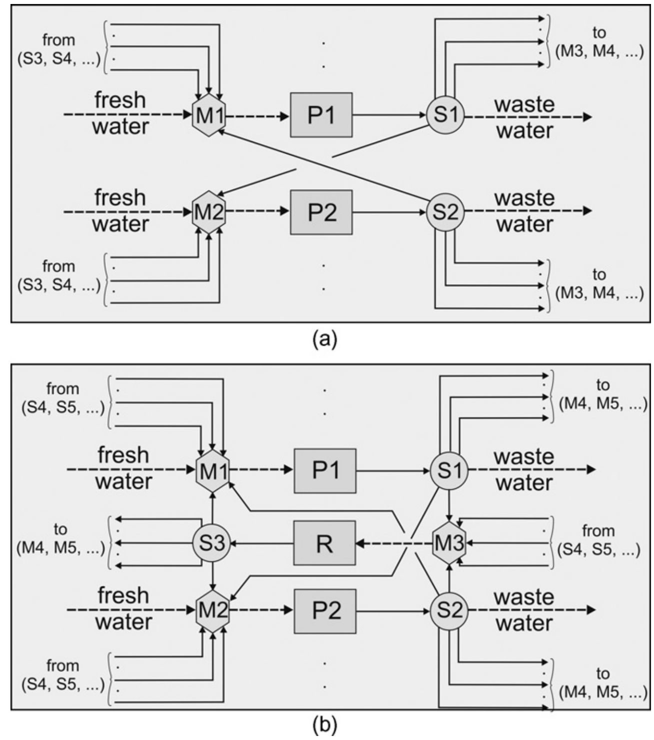

Fig. 1. (a) Simple WN superstructure for process water network synthesis. (b) WN superstructure for process water network synthesis with embedded regeneration unit.

In Fig. 2 index k refers to crossings of temperature locations in the direction of flow, rather than stages. For this reason k values coincide with stage numbers in the case of hot streams, but not in the case of cold streams. Therefore, $CF^{C}_{j,k}$ is the heat capacity flow rate of cold stream j which crossed the temperature location k. On the other hand $CF^{H}_{i,k}$ is the heat capacity flow rate of hot stream i which crossed the temperature location k. This reasoning applies to all the variables.

After hot stream i with heat capacity flow rate $CF^{H}_{i,k}$, enters stage k, it can split and send water to mix with stream i^{*} ($CF^{H'}_{i,i^{*},k}$), or

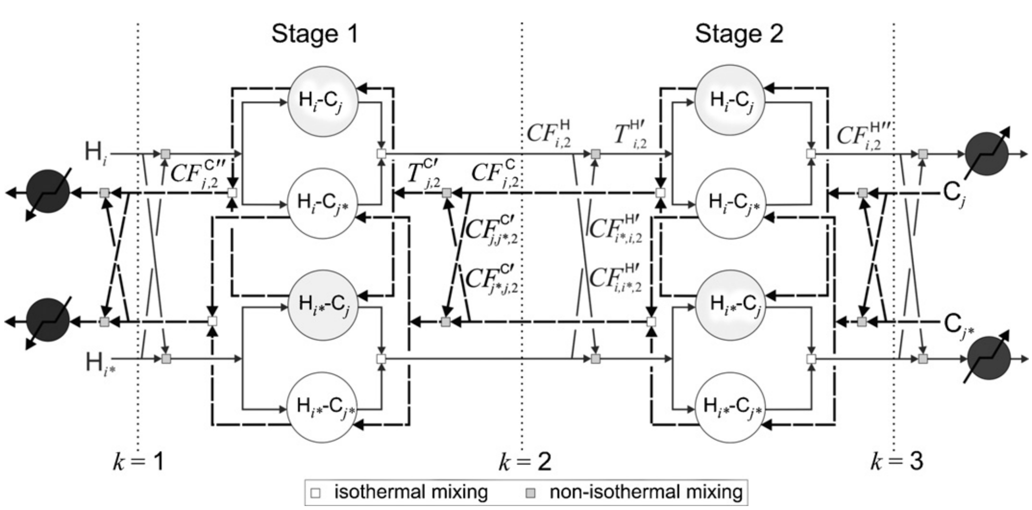

Fig. 2. Modified HEN superstructure.

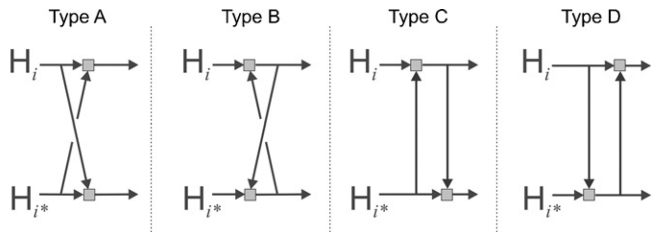

Fig. 3. Four possible types of splitting/mixing.

receive water from stream i^* ($CF^{H'}_{i^*,i,k}$). The same is allowed for cold streams. This mixing of streams can be forbidden when certain contaminants are not to be mixed. Fig. 3 shows all possible mixing/splitting patterns that one can consider. Because we expect that either mixing or splitting will take place among streams, but not both, any of these structures is appropriate. In this work Type A was chosen.

Finally, in Fig. 4 a combined superstructure, consisting of a water network (WN) superstructure (Fig. 1) and a heat exchanger network superstructure (Fig. 2) is presented.

Only certain streams (dashed lines in Fig. 4 corresponding to dashed lines in Fig. 1) are considered to take part in heat integration, that is, fresh water streams, waste water streams, and streams connecting mixer units with water using process units and mixer unit with regeneration units. Arguments supporting selection of these streams, and problems accompanying this decision are presented in the next section. Also, as discussed above, some streams are not allowed to mix within the HEN superstructure (see Fig. 4). These streams are the streams interconnecting mixer units with process units, and stream interconnecting mixer units with regeneration units.

3.1. Stream labeling

To determine whether a certain process stream is cold or hot (assuming no phase change takes place as it is in our case) one needs to know in advance its supply and target temperatures. If the temperature of the fresh water is assumed to be equal or lower than

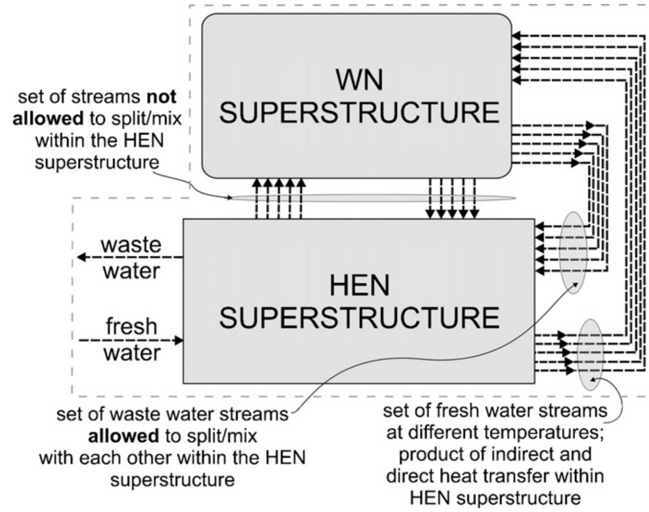

Fig. 4. Superstructure for simultaneous WN and HEN synthesis.

the lowest operating temperature of process units, each of the fresh water streams can be considered as a cold stream. In addition, if the temperature of waste water streams discharged to the environment is set to be equal or lower than the lowest operating temperature of process units, each of the waste water streams can be considered as a hot stream. Unfortunately, such unambiguous decisions are impossible to make for the rest of the streams in the water WN superstructure.

Water networks can have several alternative solutions featuring the same, minimum fresh water intake, but with different connections (Bagajewicz & Savelski, 2001). For illustration, consider the example presented in Fig. 5. Its uppermost part shows a generalized WN superstructure consisting of two process units, each operating at different temperatures. Assume that $T_{P1} > T_{P2}$ and $T_{FW} < (T_{P1}, T_{P2})$. Additionally, consider the two arbitrary selected solutions among all feasible solutions with equal fresh water intake shown in lower part of the figure. As apparent in the figure, under certain circumstances, the complicating stream connecting the mixer

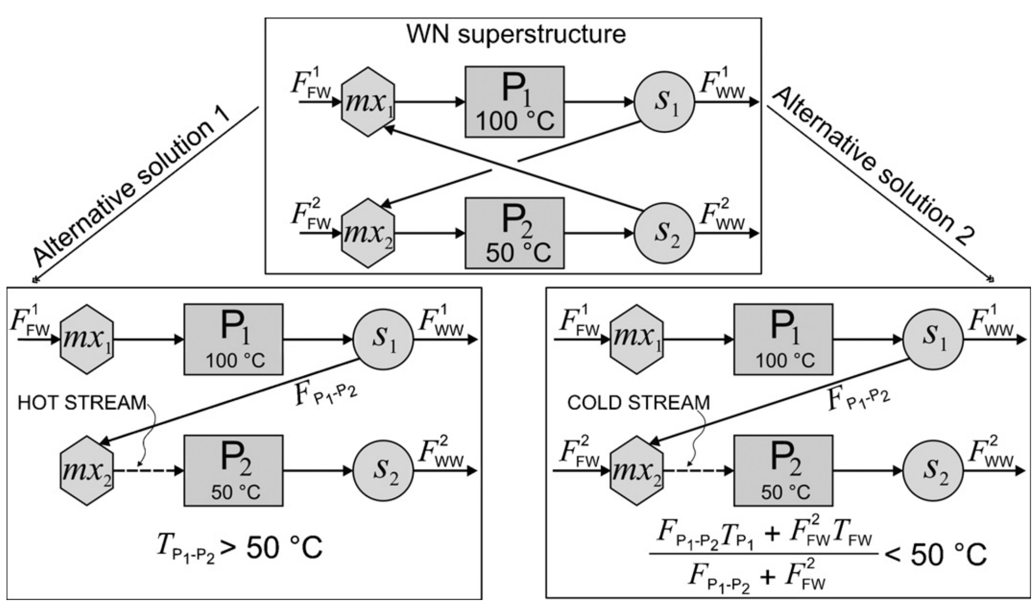

Fig. 5. Effect of alternative solutions on thermodynamic properties of streams.

unit and the process unit (dashed line) can be considered, from the perspective of the HEN, either cold or hot. Clearly, we are confronted with two issues. First, how many and which streams in the WN superstructure should be considered to take part of heat integration? In addition, on what basis should the designer decide whether the complicating streams are to be treated as hot or cold?

To make sure that the model captures the true optimal solution all, the streams in the WN superstructure should be considered for heat integration. This would most likely increase the computational effort needed. The reason for this is that the total number of streams in WN superstructure (Fig. 1a) equals N^2+3N, where N is the number of process units. In addition, since all the complicated streams (in general, all but fresh water and discharge water streams) can potentially be either cold or hot, the number of streams increases to $2(N^2+2N)$. What is more, additional logic would need to be implemented to treat these complicated streams exclusively as hot or cold. All of this would in turn make the model combinatorially very demanding. Also, it would increase the undesirable effect of non-convexities due to enlarged number of bilinear terms.

Therefore, the decision to select only the above discussed streams (dashed lines in Fig. 1) can be justified by the reduced size of the model. In addition, these streams represent the minimal number of streams that give feasible heat integrated structures and at the same time allow maximal exploitation of direct heat transfer possibilities.

4. Mathematical model

4.1. Water network model

4.1.1. Water using process units ($p\in P$) and regeneration unit ($r\in R$)

To model the water using process unit p, according to representation in Fig. 6a, we need to formulate the overall mass balance (Eq. (1)), contaminant mass balance ((Eq. (2)), and temperature inlet–outlet relation (Eq. (3)). Process unit is considered to have a single inlet stream and single outlet stream.

$$F_n = F_m \quad n\in p^{\mathrm{IN}},\ m\in p^{\mathrm{OUT}} \tag{1}$$

$$F_n c_n^l + L_p^l = F_m c_m^l \qquad p\in \mathrm{P},\ n\in p^{\mathrm{IN}},\ m\in p^{\mathrm{OUT}} \tag{2}$$

$$T_n = T_m \qquad n\in p^{\mathrm{IN}},\ m\in p^{\mathrm{OUT}} \tag{3}$$

The temperature of stream n entering the process unit p should be equal to the operating temperature of the process (T_p):

$$T_n = T_p \qquad p\in \mathrm{P},\ n\in p^{\mathrm{IN}} \tag{4}$$

When a water using process unit p is considered not to operate isothermally, its inlet and outlet temperatures are not equal, and therefore Eq. (3) becomes:

$$T_n + \Delta T_p = T_m \qquad p\in \mathrm{P},\ n\in p^{\mathrm{IN}},\ m\in p^{\mathrm{OUT}} \tag{5}$$

where $\Delta T_p\in\mathbb{R}$ is a fixed temperature change.

The constraints on maximum process inlet and outlet concentrations are:

$$c_n^l \le c_{\mathrm{IN}_{\max}p}^l \qquad p\in \mathrm{P},\ n\in p^{\mathrm{IN}} \tag{6}$$

$$c_m^l \le c_{\mathrm{OUT}_{\max}p}^l \qquad p\in \mathrm{P},\ m\in p^{\mathrm{OUT}} \tag{7}$$

As in the case of process units, a regeneration unit r is also regarded as having a single inlet and a single outlet stream (Fig. 6b). The outlet concentration of each contaminant is reduced (with respect to the inlet concentration) according to its removal efficiency η^l. The following equations model the regeneration unit r:

$$F_n = F_m \qquad n\in r^{\mathrm{IN}},\ m\in r^{\mathrm{OUT}} \tag{8}$$

$$F_n c_n^l (1-\eta^l) = F_m c_m^l \quad n\in r^{\mathrm{IN}},\ m\in r^{\mathrm{OUT}} \tag{9}$$

$$T_n = T_m \qquad n\in r^{\mathrm{IN}},\ m\in r^{\mathrm{OUT}} \tag{10}$$

In the case of a non-isothermal operation of regeneration unit r, assuming a fixed temperature change, Eq. (10) is replaced by:

$$T_n + \Delta T_r = T_m \qquad r\in R,\ n\in r^{\mathrm{IN}},\ m\in r^{\mathrm{OUT}} \tag{11}$$

A mixer unit ($mx\in \mathrm{M}$) is shown in Fig. 7a, having multiple inlet streams ($(n, fw)\in mx^{\mathrm{IN}}$) and a single outlet stream ($m\in mx^{\mathrm{OUT}}$). The index fw is associated with a single fresh water stream, and index n with all the other streams (coming from splitter units ($s\in \mathrm{S}$)). The overall mass balance is given by Eq. (12), the individual contaminant balances by Eq. (13), and the energy balance by Eq. (14).

In turn, a splitter unit ($s\in \mathrm{S}$) is depicted in Fig. 7b, consisting of a single inlet stream ($n\in s^{\mathrm{IN}}$) and multiple outlet streams, namely streams $m\in s^{\mathrm{OUT}}$ linked to mixer units ($mx\in \mathrm{M}$), and a single waste water discharge stream $ww\in s^{\mathrm{OUT}}$. Splitter units are modeled using Eqs. ((15)–(19)).

4.1.2. Mixer units ($mx\in M$)

$$F_m = \sum_n F_n + F_{fw} \qquad m\in mx^{\mathrm{OUT}}, \quad (n, fw)\in mx^{\mathrm{IN}} \tag{12}$$

$$F_m c_m^l = \sum_n F_n c_n^l \qquad m\in mx^{\mathrm{OUT}}, n\in mx^{\mathrm{IN}} \tag{13}$$

$$F_m T_m = \sum_n F_n T_n + F_{fw} T_{fw} \qquad m\in mx^{\mathrm{OUT}}, (n, fw)\in mx^{\mathrm{IN}} \tag{14}$$

4.1.3. Splitter units ($s\in S$)

$$F_n = \sum_m F_m + F_{ww} \qquad (m, ww)\in s^{\mathrm{OUT}}, n\in s^{\mathrm{IN}} \tag{15}$$

$$c_n^l = c_m^l \qquad m\in s^{\mathrm{OUT}}, n\in s^{\mathrm{IN}} \tag{16}$$

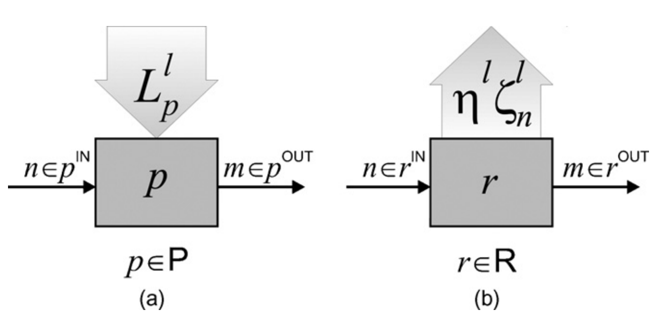

Fig. 6. (a) Schematic representation of process unit. (b) Schematic representation of regeneration unit.

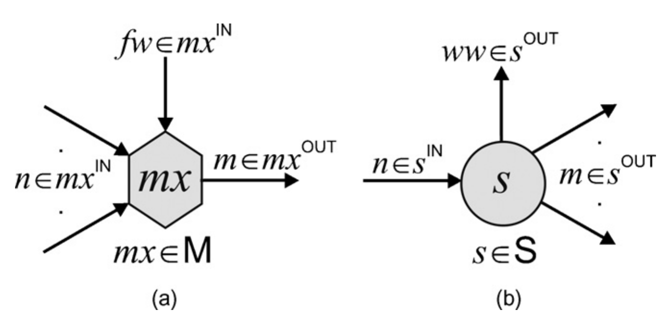

Fig. 7. (a) Schematic representation of mixer unit. (b) Schematic representation of splitter unit.

$$c_n^l = c_{ww}^l \qquad ww \in s^{\mathrm{OUT}}, n \in s^{\mathrm{IN}} \tag{17}$$

$$T_n = T_m \qquad m \in s^{\mathrm{OUT}}, n \in s^{\mathrm{IN}} \tag{18}$$

$$T_n = T_{ww} \qquad ww \in s^{\mathrm{OUT}}, n \in s^{\mathrm{IN}} \tag{19}$$

Note that a mixer unit and a splitter unit linked to a regeneration unit (see Fig. 1b) differ from the rest of the mixer and splitter units. The former does not have the fresh water feed while the latter does not have the waste water discharge stream. The formulation of this mixer unit is straightforward: only the variables associated with fresh water stream need to be excluded from Eqs. (12) and (14). For the splitter unit, the flow rate of the discharged waste water stream (F_{ww}) is excluded from the formulation of the overall mass balance (Eq. (15)), and Eqs. (17) and (19) become redundant.

4.2. HEN model

As described above, for this model, we extend the MINLP formulation of Yee and Grossmann (1990) by adding mixing at each stage. The first main difference between the original stage-wise formulation and the proposed one is additional continuous variables needed to model the non-isothermal mixing in each stage. Note that even when inlet heat capacity flow rates ($CF_i^{\mathrm{H,IN}}$, $CF_j^{\mathrm{C,IN}}$) and inlet/outlet temperatures are fixed the new energy balance introduces several additional bilinear terms adding to the model non-convexity. Also, the overall heat balance of each stream is not explicitly stated because there is splitting and mixing taking place. The overall heat balance is, nonetheless, satisfied.

4.2.1. Assignment of superstructure inlet temperatures and inlet heat capacity flow rates

$$T_i^{\mathrm{H,IN}} = T_{i,1}^{\mathrm{H}} \qquad i \in \mathrm{HP} \tag{20}$$

$$T_j^{\mathrm{C,IN}} = T_{j,\mathrm{NOK}+1}^{\mathrm{C}} \qquad j \in \mathrm{CP} \tag{21}$$

$$CF_i^{\mathrm{H,IN}} = CF_{i,1}^{\mathrm{H}} \qquad i \in \mathrm{HP} \tag{22}$$

$$CF_j^{\mathrm{C,IN}} = CF_{j,\mathrm{NOK}+1}^{\mathrm{C}} \qquad j \in \mathrm{CP} \tag{23}$$

4.2.2. Stage heat balance for hot and cold streams

$$(T_{i,k}^{\mathrm{H}'} - T_{i,k+1}^{\mathrm{H}})CF_{i,k}^{\mathrm{H}''} = \sum_{j \in \mathrm{CP}} q_{i,j,k} \qquad k \in \mathrm{ST},\ i \in \mathrm{HP} \tag{24}$$

$$(T_{j,k}^{\mathrm{C}} - T_{j,k+1}^{\mathrm{C}'})CF_{j,k+1}^{\mathrm{C}''} = \sum_{i \in \mathrm{HP}} q_{i,j,k} \qquad k \in \mathrm{ST}, j \in \mathrm{CP} \tag{25}$$

4.2.3. Cold and hot utility load

$$q_{\mathrm{CU}\,i} = CF_{i,\mathrm{NOK}+1}^{\mathrm{H}''}(T_{i,\mathrm{NOK}+1}^{\mathrm{H}'} - T_i^{\mathrm{H,OUT}}) \qquad i \in \mathrm{HP} \tag{26}$$

$$q_{\mathrm{HU}\,j} = CF_{j,1}^{\mathrm{C}''}(T_j^{\mathrm{C,OUT}} - T_{j,1}^{\mathrm{C}'}) \qquad j \in \mathrm{CP} \tag{27}$$

4.2.4. Stage heat capacity flow rate balances for hot and cold streams

$$CF_{i,k}^{\mathrm{H}} + \sum_{i*} CF_{i*,i,k}^{\mathrm{H}'} - \sum_{i*} CF_{i,i*,k}^{\mathrm{H}'} = CF_{i,k}^{\mathrm{H}''}$$

$$k \in \mathrm{ST} \cup \mathrm{NOK}+1,\ i \in \mathrm{HP} \wedge i \neq i^* \tag{28}$$

$$CF_{j,k}^{\mathrm{C}} + \sum_{j*} CF_{j*,j,k}^{\mathrm{C}'} - \sum_{j*} CF_{j,j*,k}^{\mathrm{C}'} = CF_{j,k}^{\mathrm{C}''}$$

$$k \in \mathrm{ST} \cup \mathrm{NOK}+1,\ j \in \mathrm{CP} \wedge j \neq j^* \tag{29}$$

4.2.5. Stage enthalpy balances for hot and cold streams

$$CF_{i,k}^{\mathrm{H}} T_{i,k}^{\mathrm{H}} + \sum_{i*} CF_{i*,i,k}^{\mathrm{H}'} T_{i*,k}^{\mathrm{H}} - \sum_{i*} CF_{i,i*,k}^{\mathrm{H}'} T_{i,k}^{\mathrm{H}} = CF_{i,k}^{\mathrm{H}''} T_{i,k}^{\mathrm{H}'}$$

$$k \in \mathrm{ST} \cup \mathrm{NOK}+1,\ i \in \mathrm{HP} \wedge i \neq i^* \tag{30}$$

$$CF_{j,k}^{\mathrm{C}} T_{j,k}^{\mathrm{C}} + \sum_{j*} CF_{j*,j,k}^{\mathrm{C}'} T_{j*,k}^{\mathrm{C}} - \sum_{j*} CF_{j,j*,k}^{\mathrm{C}'} T_{j,k}^{\mathrm{C}} = CF_{j,k}^{\mathrm{C}''} T_{j,k}^{\mathrm{C}'}$$

$$k \in \mathrm{ST} \cup \mathrm{NOK}+1,\ i \in \mathrm{CP} \wedge j \neq j^* \tag{31}$$

Note that the Eqs. (28)–(31) are not restricted to $k \in \mathrm{ST}$. Since, for example, mixing of hot streams is possible even after the crossing of last temperature location ($k=3$ in Fig. 2), the equations should hold also for $k+1$ (NOK + 1). The same is true cold streams.

4.2.6. Overall stage heat capacity flow rate balance

$$\sum_i CF_{i,k}^{\mathrm{H}} = \sum_i CF_{i,k}^{\mathrm{H}''} \qquad i \in \mathrm{HP},\ k \in \mathrm{ST} \cup \mathrm{NOK}+1 \tag{32}$$

$$\sum_j CF_{j,k}^{\mathrm{C}} = \sum_j CF_{j,k}^{\mathrm{C}''} \qquad j \in \mathrm{CP},\ k \in \mathrm{ST} \cup \mathrm{NOK}+1 \tag{33}$$

4.2.7. Bounds on splits (non-isothermal mixing)

$$\sum_{i*} CF_{i,i*,k}^{\mathrm{H}'} \le CF_{i,k}^{\mathrm{H}} \qquad i \in \mathrm{HP} \wedge i \neq i^*, k \in \mathrm{ST} \cup \mathrm{NOK}+1 \tag{34}$$

$$\sum_{j*} CF_{j,j*,k}^{\mathrm{C}'} \le CF_{j,k}^{\mathrm{C}} \qquad j \in \mathrm{CP} \wedge j \neq j^*, k \in \mathrm{ST} \cup \mathrm{NOK}+1 \tag{35}$$

4.2.8. Stage inlet and outlet heat capacity flow rate relation

$$CF_{i,k+1}^{\mathrm{H}} = CF_{i,k}^{\mathrm{H}''} \qquad i \in \mathrm{HP},\ k \in \mathrm{ST} \tag{36}$$

$$CF_{j,k}^{\mathrm{C}} = CF_{j,k+1}^{\mathrm{H}''} \qquad j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{37}$$

4.2.9. Logical constraints needed to determine the existence of a heat exchange match (i,j) in stage k

$$q_{i,j,k} - \Omega z_{i,j,k} \le 0 \qquad i \in \mathrm{HP},\ j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{38}$$

$$q_{\mathrm{CU}\,i} - \Omega_{\mathrm{CU}} z_{\mathrm{CU}\,i} \le 0 \qquad i \in \mathrm{HP} \tag{39}$$

$$q_{\mathrm{HU}\,j} - \Omega_{\mathrm{HU}} z_{\mathrm{HU}\,j} \le 0 \qquad j \in \mathrm{CP} \tag{40}$$

4.2.10. Logical constraints activating temperature differences in stage k

$$\Delta T_{i,j,k}^{\mathrm{H}} \le T_{i,k}^{\mathrm{H}'} - T_{j,k}^{\mathrm{C}} + \Gamma(1 - z_{i,j,k}) \qquad i \in \mathrm{HP}, j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{41}$$

$$\Delta T_{i,j,k}^{\mathrm{C}} \le T_{i,k+1}^{\mathrm{H}} - T_{j,k+1}^{\mathrm{C}'} + \Gamma(1 - z_{i,j,k}) \quad i \in \mathrm{HP},\ j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{42}$$

$$\Delta T_{\mathrm{CU}\ i} \le T_{i,\mathrm{NOK}+1}^{\mathrm{H}'} - T_{\mathrm{CU}}^{\mathrm{OUT}} + \Gamma(1 - z_{\mathrm{CU}\,i}) \qquad i \in \mathrm{HP} \tag{43}$$

$$\Delta T_{\mathrm{HU}\ j} \le T_{\mathrm{HU}}^{\mathrm{OUT}} - T_{j,1}^{\mathrm{C}'} + \Gamma(1 - z_{\mathrm{HU}\,j}) \qquad j \in \mathrm{CP} \tag{44}$$

The above four constraints can be expressed as inequalities because the costs of heat exchangers decrease with the increase in the temperature differences. And since the objective function is to be minimized, the temperatures will be driven to take the highest possible value. The role of binaries in these constraints is to ensure positive driving forces.

4.2.11. Lower bounds on temperature differences

$$\Delta T_{\mathrm{H}\,i,j,k} \ge \mathrm{EMAT} \qquad i \in \mathrm{HP}, j \in \mathrm{CP}, k \in \mathrm{ST} \tag{45}$$

$$\Delta T_{\mathrm{C}\ i,j,k} \ge \mathrm{EMAT} \qquad i \in \mathrm{HP},\ j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{46}$$

$$\Delta T_{\mathrm{CU}\ i} \ge \mathrm{EMAT} \qquad i \in \mathrm{HP} \tag{47}$$

$$\Delta T_{\mathrm{HU}\,j} \ge \mathrm{EMAT} \qquad j \in \mathrm{CP} \tag{48}$$

4.2.12. Feasibility of temperatures

$$T^{H'}_{i,NOK+1} \geq T^{H,OUT}_{i} \qquad i \in HP \tag{49}$$

$$T^{H'}_{i,k} \geq T^{H}_{i,k+1} \qquad i \in HP, \quad k \in ST \tag{50}$$

$$T^{C'}_{j,1} \leq T^{C,OUT}_{j} \qquad j \in CP \tag{51}$$

$$T^{C'}_{j,k+1} \leq T^{C}_{j,k} \qquad j \in CP, \quad k \in ST \tag{52}$$

$$T^{H'}_{i,k} \leq \max\{0, T^{H,IN}_{i}\} \qquad i \in HP \tag{53}$$

$$T^{C'}_{j,k} \geq \min\{c, T^{C,IN}_{j}\} \qquad j \in CP, (c \in \mathbb{R}^{+} \wedge c \gg T^{C,IN}_{j}) \tag{54}$$

Monotonic decrease of temperature at each successive stage for each stream is not requested and expected to take place in this formulation. However, monotonic decrease within each stage is enforced through Eqs. (49)–(52). Also, note that the valid upper bound on temperatures for hot streams, which are allowed to mix, is the inlet temperature of the hottest hot stream (Eq. (53)). Likewise, the valid lower bound on temperatures for the cold streams, which are also allowed to mix, is the inlet temperature of the coldest stream (Eq. (54)).In turn, *forbidden stream splitting and mixing* can be achieved by the following set of constraints:

$$CF^{H'}_{i,i^*,k} = 0 \qquad i \in HP \wedge i \neq i^*, \quad k \in ST \cup NOK+1 \tag{55}$$

$$CF^{H'}_{i^*,i,k} = 0 \qquad i \in HP \wedge i \neq i^*, k \in ST \cup NOK+1 \tag{56}$$

$$CF^{C'}_{j,j^*,k} = 0 \qquad j \in HP \wedge j \neq j^*, \quad k \in ST \cup NOK+1 \tag{57}$$

$$CF^{C'}_{j^*,j,k} = 0 \qquad j \in HP \wedge j \neq j^*, k \in ST \cup NOK+1 \tag{58}$$

The constraints represented by Eqs. (55)–(58) (i.e. fixing the values of the variables to zero) are the simplest way to enforce forbidden mixing/splitting of streams in the HEN superstructure. However, this formulation gives the designer no control over the number of splits and their heat capacity flow rates. For example, from strictly practical reasons, one may want to impose some lower and upper bounds on the heat capacity flow rates of splits, essentially setting bounds on water flow rates of splits. Furthermore, to obtain a less complex HEN topology it is beneficial to limit the number of splits in each stage. This can be done through the following constraints:

$$CF^{H'}_{i,i^*,k} \geq CF^{H,LO} y^{H}_{i,i^*,k} \tag{59}$$

$$CF^{H'}_{i,i^*,k} \leq CF^{H,UP} y^{H}_{i,i^*,k} \tag{60}$$

$$y^{H}_{i,i^*,k} + y^{H}_{i^*,i,k} \leq 1 \tag{61}$$

$(CF^{H,LO}, CF^{H,UP}) \in \mathbb{R}^{+}$
$y^{H}_{i,i,k} \in \{0, 1\}$
$i \in HP \wedge i \neq i^*, k \in ST \cup NOK+1$

$$CF^{C'}_{j,j*,k} \geq CF^{C,LO} y^{C}_{j,j^*,k} \tag{62}$$

$$CF^{C'}_{j,j*,k} \leq CF^{C,UP} y^{C}_{j,j^*,k} \tag{63}$$

$$y^{C}_{j,j^*,k} + y^{C}_{j^*,j,k} \leq 1 \tag{64}$$

$(CF^{C,LO}, CF^{C,UP}) \in \mathbb{R}^{+}$
$y^{C}_{j,j,k} \in \{0, 1\}$
$j \in HP \wedge j \neq j^*, k \in ST \cup NOK+1$

Using the above formulation the following effects on the HEN topology is achieved.

- *Bounds on splitting flow rates:* Eqs. (59) and (60) state that if the binary variable $y^{H}_{i,i^*,k}$ equals one in stage k, then splits $CF^{H'}_{i,i^*,k}$ of hot stream i can take some value between lower and upper bounds ($CF^{H,LO}$, $CF^{H,UP}$). Otherwise, splits are forced to zero.
- *Limitation on the number of split streams:* If a single split $CF^{H'}_{i,i^*,k}$ exists in stage k, then the all the splits $CF^{H'}_{i^*,i,k}$ in this stage are forced to zero – inequality constraint on binary variable (Eq. (61)). The same is true for splits of cold streams ($CF^{C'}_{j,j^*,k}$, $CF^{C'}_{j^*,j,k}$), Eqs. ((62)–(64)).

Also note that all of the types of mixing depicted in Fig. 3 are represented by Eqs. (59)–(64) because cross-mixing is excluded.

4.3. Constraints connecting the WN and the HEN

4.3.1. Fresh water streams

The temperature of fresh water source (T^{FWS}) is assumed to be fixed, therefore, the inlet temperatures of fresh water streams can be treated as parameters.

$$T^{C,IN}_{j} = T^{FWS} \qquad j \in CP \tag{65}$$

On the other hand, their heat capacity flow rates ($CF^{C,IN}_{j}$) are variables whose values are to be determined by solving the combined WN–HEN model.

$$CF^{C,IN}_{j} = CF^{C}_{j,NOK+1} \qquad j \in CP \tag{66}$$

$$T^{C,OUT}_{j} = T_{fw} \qquad fw \in mx^{IN}, \ mx \in M, \ j \in CP \tag{67}$$

$$CF^{C''}_{j,1} = F_{fw} Cp \qquad n \in mx^{IN}, mx \in M, \ j \in CP \tag{68}$$

4.3.2. Streams connecting mixer units ($mx \in M$) to process units ($p \in P$), and mixer unit ($mx \in M$) to regeneration unit ($r \in R$)

For the streams considered as cold streams the variables in HEN superstructure and WN superstructure are related through equations:

$$T^{C,IN}_{j} = T_{m} \qquad m \in mx^{OUT}, \ mx \in M, \ j \in CP \tag{69}$$

$$CF^{C,IN}_{j} = F_{m} Cp \qquad m \in mx^{OUT}, mx \in M, \ j \in CP \tag{70}$$

$$T^{C,OUT}_{j} = T_{n} \qquad n \in p^{IN}, n \in r^{IN}, \ p \in P, r \in R, \ j \in CP \tag{71}$$

$$CF^{C''}_{j,1} = F_{n} Cp \qquad n \in p^{IN}, n \in r^{IN}, \ p \in P, r \in R, \ j \in CP \tag{72}$$

In contrast, for the streams considered as hot streams the following equations are used:

$$T^{H,IN}_{i} = T_{m} \qquad m \in mx^{OUT}, \ mx \in M, \ i \in HP \tag{73}$$

$$CF^{H,IN}_{i} = F_{m} Cp \qquad m \in mx^{OUT}, mx \in M, \ i \in HP \tag{74}$$

$$T^{H,OUT}_{i} = T_{n} \qquad n \in p^{IN}, n \in r^{IN}, \ p \in P, r \in R, \ i \in HP \tag{75}$$

$$CF^{H''}_{i,NOK+1} = F_{n} Cp \qquad n \in p^{IN}, n \in r^{IN}, \ p \in P, r \in R, \ j \in CP \tag{76}$$

Regardless of whether these streams are hot or cold, equations to make the concentrations of contaminants and flow rates of streams leaving the mixer units (streams entering the HEN superstructure) equal to the ones in the streams feeding the process units or the regeneration unit (streams leaving the HEN superstructure) are needed. They are the following:

$$F_{m} = F_{n} \qquad m \in mx^{OUT}, \ n \in p^{IN}, \ n \in r^{IN} mx \in M, \ p \in P, \ r \in R \tag{77}$$

$$c^{l}_{m} = c^{l}_{n} \qquad m \in mx^{OUT}, \ n \in p^{IN}, \ n \in r^{IN} \ mx \in M, \ p \in P, \ r \in R \tag{78}$$

4.3.3. Waste water discharge streams

$$T_i^{\mathrm{H,IN}} = T_{ww} \qquad ww \in s^{\mathrm{OUT}},\ s \in \mathrm{S},\ i \in \mathrm{HP} \tag{79}$$

$$CF_i^{\mathrm{H,IN}} = F_{ww}Cp \qquad ww \in s^{\mathrm{OUT}}, s \in S,\ i \in \mathrm{HP} \tag{80}$$

The outlet temperature of all the discharge waste water streams is assumed to be equal to the temperature of waste water sink (T^{WWS}):

$$T_j^{\mathrm{H,OUT}} = T^{\mathrm{WWS}} \qquad i \in \mathrm{HP} \tag{81}$$

4.4. Objective function

The annualized cost of the HEN, comprising annual utility costs and investment costs is:

$$\begin{aligned} C_{\mathrm{a}}^{\mathrm{HEN}} = & \sum_{i \in \mathrm{HP}}\sum_{j \in \mathrm{CP}}\sum_{k \in \mathrm{ST}} C_{\mathrm{HE}\ i,j} z_{i,j,k} + \sum_{i \in \mathrm{HP}} C_{\mathrm{HE}\ i} z_{\mathrm{CU}\,i} \\ & + \sum_{j \in \mathrm{CP}} C_{\mathrm{HE}\,j} z_{\mathrm{HU}\,j} + f_{\mathrm{a}} \left(\sum_{i \in \mathrm{HP}} C_{\mathrm{CU}} q_{\mathrm{CU}\,i} + \sum_{j \in \mathrm{CP}} C_{\mathrm{HU}} q_{\mathrm{HU}\,j} \right) \\ & + \sum_{i \in \mathrm{HP}}\sum_{j \in \mathrm{CP}}\sum_{k \in \mathrm{ST}} C_{\mathrm{A}\ i,j} A_{i,j,k}^{\beta} + \sum_{i \in \mathrm{HP}} C_{\mathrm{A}\,i} A_{\mathrm{CU}\,i}^{\beta} + \sum_{j \in \mathrm{CP}} C_{\mathrm{A}\,j} A_{\mathrm{HU}\ j}^{\beta} \\ & + C_{\mathrm{CON}} \left(\sum_{i \in \mathrm{HP}} \sum_{\substack{i^* \in \mathrm{HP} \\ i^* \neq i}} \sum_{k \in \mathrm{ST}} y_{i,i^*,k}^{\mathrm{H}} + \sum_{j \in \mathrm{CP}} \sum_{\substack{j^* \in \mathrm{CP} \\ j^* \neq j}} \sum_{k \in \mathrm{ST}} y_{j,j^*,k}^{\mathrm{C}} \right) \end{aligned} \tag{82}$$

where f_{a} is the time fraction of operation in a year. The areas and heat transfer coefficients, in turn, are given by the following standard relations:

$$A_{i,j,k} = \frac{q_{i,j,k}}{U_{i,j} \times \Delta_{\ln} T_{i,j,k}} \qquad i \in \mathrm{HP},\ j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{83}$$

$$A_{\mathrm{CU}\ i} = \frac{q_{\mathrm{CU}\,i}}{U_{i,\mathrm{CU}} \times \Delta_{\ln} T_{i,\mathrm{CU}}} \qquad i \in \mathrm{HP} \tag{84}$$

$$A_{\mathrm{HU}\ j} = \frac{q_{\mathrm{HU}\,i}}{U_{j,\mathrm{HU}} \times \Delta_{\ln} T_{j,\mathrm{HU}}} \qquad j \in \mathrm{CP} \tag{85}$$

$$\frac{1}{U_{i,j}} = \frac{1}{h_i} + \frac{1}{h_j} \qquad i \in \mathrm{HP},\ j \in \mathrm{CP} \tag{86}$$

$$\frac{1}{U_{i,\mathrm{CU}}} = \frac{1}{h_i} + \frac{1}{h_{\mathrm{CU}}} \qquad i \in \mathrm{HP} \tag{87}$$

$$\frac{1}{U_{j,\mathrm{HU}}} = \frac{1}{h_j} + \frac{1}{h_{\mathrm{HU}}} \qquad j \in \mathrm{CP} \tag{88}$$

Finally, the logarithmic mean temperature difference ($\Delta_{\ln} T$) is approximated according to Chen (1987):

$$\Delta_{\ln} T_{i,j,k} = \left(\Delta T_{\mathrm{H}\ i,j,k} \times \Delta T_{\mathrm{C}\ i,j,k} \times \frac{(\Delta T_{\mathrm{H}\ i,j,k} + \Delta T_{\mathrm{C}\ i,j,k})}{2} \right)^{1/3} \quad i \in \mathrm{HP},\ j \in \mathrm{CP},\ k \in \mathrm{ST} \tag{89}$$

$$\Delta_{\ln} T_{i,\mathrm{CU}} = \left(\Delta T_{\mathrm{CU}\,i} (T_i^{\mathrm{OUT}} - T_{\mathrm{CU}}^{\mathrm{IN}}) \frac{(\Delta T_{\mathrm{CU}\,i} + (T_i^{\mathrm{OUT}} - T_{\mathrm{CU}}^{\mathrm{IN}}))}{2} \right)^{1/3} \quad i \in \mathrm{HP} \tag{90}$$

$$\Delta_{\ln} T_{j,\mathrm{HU}} = \left(\Delta T_{\mathrm{HU}\,j} \times (T_{\mathrm{HU}}^{\mathrm{IN}} - T_j^{\mathrm{OUT}}) \frac{(\Delta T_{\mathrm{HU}\,j} + (T_{\mathrm{HU}}^{\mathrm{IN}} - T_j^{\mathrm{OUT}}))}{2} \right)^{1/3} \quad j \in \mathrm{CP} \tag{91}$$

The last term of the objective function represents the fixed costs associated to splits of hot and cold streams. One can justify this by the capital costs of additional equipment (valves, regulation, etc.) needed to operate the HEN.

The annualized WN costs are given by:

$$C_{\mathrm{a}}^{\mathrm{WN}} = N_h f_{\mathrm{a}} \left(C_{\mathrm{FW}} \sum_{fw} F_{fw} + C_{\mathrm{R}} F_{\mathrm{n}} \right) + C_{\mathrm{R,v}} F_n^{\alpha} \qquad fw \in mx^{\mathrm{IN}},\ n \in r^{\mathrm{IN}} \tag{92}$$

where N_h is the number of hours in a year. While the first term of the WN objective function (Eq. (92)) corresponds to operating costs of WN, namely to fresh water and regeneration costs, the last term corresponds to variable costs associated with regeneration unit capacity.

5. Solution procedure

To overcome the ambiguity caused by the need of labeling streams as hot or cold we propose the following strategy:

Step 1: The WN model was solved using a local NLP solver. However, prior to solving the WN model a minor reformulation is needed. Indeed, to meet the target process operating temperatures, positive slack variables $\varsigma_{mx}^{\mathrm{CU}}$ and $\varsigma_{mx}^{\mathrm{HU}}$ representing external heating and cooling are added into the formulation of the mixer unit energy balance. Then, Eq. (14) becomes:

$$F_m T_m + \varsigma_{mx}^{\mathrm{HU}} - \varsigma_{mx}^{\mathrm{CU}} = \sum_{n \in mx_{\mathrm{in}}} F_n T_n \qquad \forall mx \in \mathrm{M},\ m \in mx^{\mathrm{OUT}} \tag{93}$$

The WN objective function (Eq. (92)) is reformulated including the slack variables and adding a small price (π) to them.

$$\begin{aligned} C_{\mathrm{a}}^{\mathrm{WN}} = & N_h f_{\mathrm{a}} \left(C_{\mathrm{FW}} \sum_{\mathrm{fw}} F_{fw} + C_{\mathrm{R}} F_n \right) + C_{\mathrm{R,v}} F_n^{\alpha} \\ & + \pi \sum_{mx} (\varsigma_{mx}^{\mathrm{HU}} + \varsigma_{mx}^{\mathrm{CU}}) \end{aligned} \tag{94}$$

The above objective function minimizes the water related cost, but equally important, it tends to maximize the direct heat transfer in mixer units by minimizing the values of the slack variables. Also important is that due to small prices assigned to the slack variables the possibility of both having positive value in a particular mixer unit is excluded. In addition, both variables can take the value of zero.

Labeling of the complicated streams is then performed according to the values of the slack variables in the solution of the reformulated WN model. First, if variable $\varsigma_{mx}^{\mathrm{HU}}$ takes a positive value then the stream connecting a mixer unit with a process unit is considered to be cold, because additional heating is needed to achieve its target temperature. On the other hand, if the value of $\varsigma_{mx}^{\mathrm{CU}}$ is greater than zero the stream is considered a hot stream. When both the slack variables are zero, the stream is not considered to take part in heat integration, since its target temperature is met by direct heat transfer in the corresponding mixer unit.

Step 2: Solve the combined WN–HEN model. According to our experiences the values of continuous variables (flow rates,

Table 1
Cost and operating parameters for WN and HEN

Parameter		Parameter		Parameter	
C_{CON} (\$)	3×10^3	C_{HU} (\$/(kW a))	260	T_{HU}^{IN}(°C)	126
C_{HE} (\$)	10×10^3	C_{CU} (\$/(kW a))	150	T_{HU}^{OUT}(°C)	126
C_A (\$/m^2)	860	C_{FW} (\$/t)	2.5	T_{CU}^{IN}(°C)	15
β/1	0.75	C_R (\$/t)	0.95	T_{CU}^{OUT}(°C)	20
α/1	0.78	$C_{R,v}$ (\$ h/t)	20×10^3		

$h_{CP,HP,CU}$ (kW/(m^2 K)) = 1, h_{HU} (kW/(m^2 K)) = 5, $CF^{(C,H),LO}$ (kW/K) = 1.163.

temperatures, etc.) obtained in the solution of the reformulated WN model serve as a good initial guess for the assignment of the HEN superstructure inlet conditions.

6. Examples

Four examples are given in this section to illustrate the proposed approach. In all of the examples the same cost factors, inlet/outlet utility temperatures were used (Table 1). The lower bound on splits are 1 t/h and the time fraction of operation in a year, f_a = 0.95, was assumed in all cases. Also, in all of the examples the fresh water temperature is 20 °C, and the discharge temperature of waste water is 30 °C.

Finally, the examples were implemented in GAMS (Brooke, Kendrick, Meeraus, & Raman, 1998) and solved using DICOPT (Viswanathan & Grossmann, 1990) with CPLEX as a MIP solver and SNOPT (Gill, Murray, & Saunders, 2002) as a NLP solver on a PC machine (3.2 GHz, 1 GB RAM).

To reduce the problems caused by infeasible NLP sub-problems, the combined model was reformulated using the integer-infeasible path strategy (Soršak & Kravanja, 2002). The reformulation was performed only on the binary variables assigned to determine the heat exchange matches ($z_{i,j,k}$, $z_{CU\,i}$, $z_{HU\,j}$).

Table 2
Data for example 1

Process	L^l (kg/h)	c_{max}^{IN}(mg/kg)	c_{max}^{OUT}(mg/kg)/	T_p (°C)
P1	7.2	0	100	40
P2	18.0	50	100	100
P3	108.0	50	800	75
P4	14.4	400	800	50

Table 3
Data for example 2

Process	L^l (kg/h)	c_{max}^{IN}(mg/kg)	c_{max}^{OUT}(mg/kg)	T_p (°C)
P1	2	0	100	40
P2	5	50	100	100
P3	30	50	800	75
P4	4	400	800	50

6.1. Example 1

The first example is the one originally proposed by Savulescu and Smith (1998); a single-contaminant case comprising four water using process units. The data is presented in Table 2.

To be able to compare results with solutions obtained by Savulescu et al. (2005b) and Bagajewicz et al. (2002) the heat exchanger network was designed exclusively using fresh water and discharge waste water streams without considering the process to process streams. The network obtained using the proposed approach with annual operating costs of 7.671 M\$/a and HEN capital cost of 0.622 M\$ is depicted in Fig. 8. The corresponding HEN consists of three heat exchangers featuring a total area of 3498.4 m^2, and a single heater (132.2 m^2). Fresh water intake equals 324 t/h.

The network presented in Fig. 8 is identical to the one reported in Bagajewicz et al. (2002). The solution obtained by Savulescu et al. (2005b) is depicted in Fig. 9; the authors used a systematic

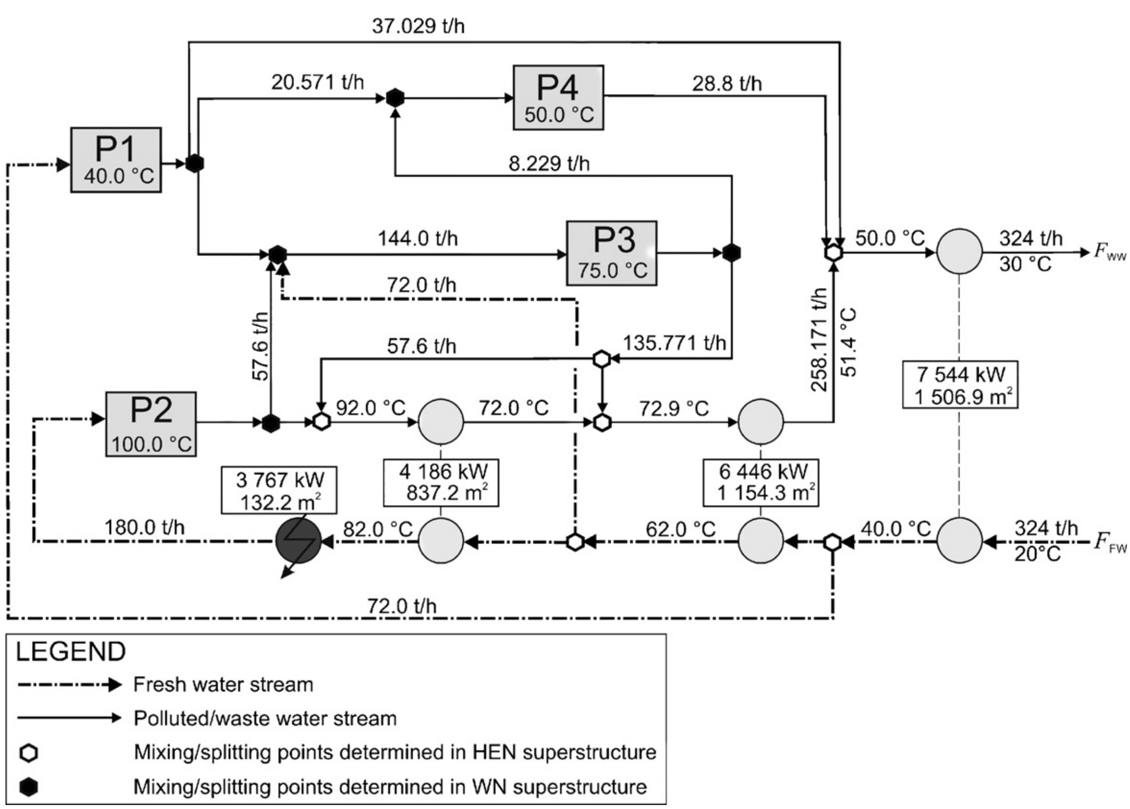

Fig. 8. Heat integrated water network for example 1.

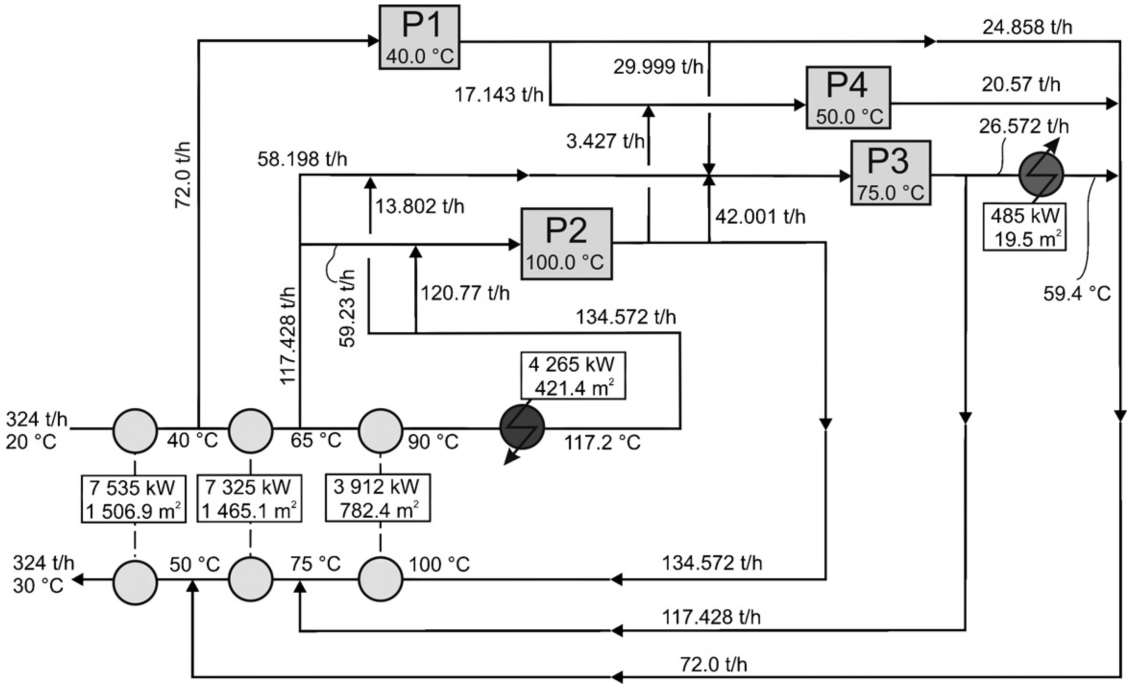

Fig. 9. Solution of example 1 by Savulescu et al. (2005b).

conceptual approach aiming to simplify the network topology by considering non-isothermal mixing.

Because not enough information was given in the original paper, the areas of the heat exchanger of Fig. 9 were calculated using the data of Table 1. Clearly, the fresh water intake is identical as in the above presented solution (see Fig. 8), but, the HEN is different. Note that the total area of the three heat exchangers is approximately 7% larger than the one obtained using our approach. Also, besides the 13% larger hot utility consumption, 485 kW of cold utility is needed.

Summarizing, the solution obtained using our proposed approach is found to be superior to the one reported by Savulescu

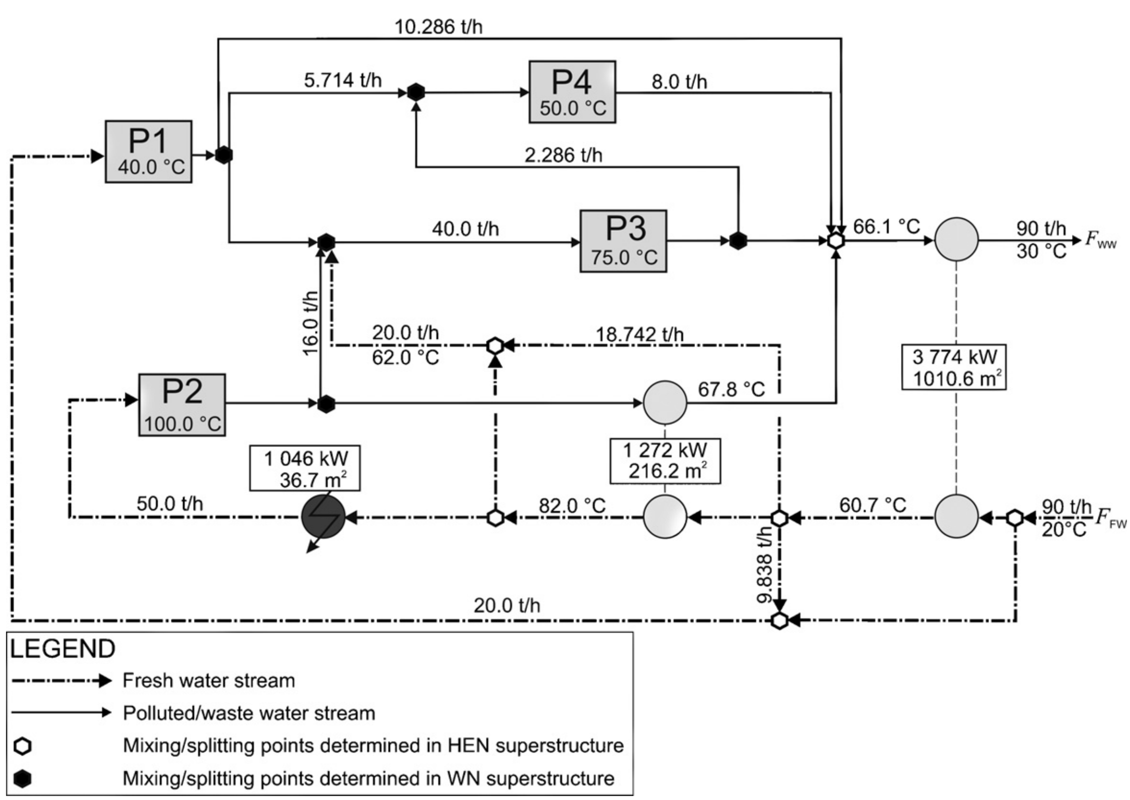

Fig. 10. Heat integrated water network for example 2.

Table 4
Data for example 3

Process	L^I (kg/h)			c_{max}^{IN}(mg/kg)			c_{max}^{OUT}(mg/kg)			T_p (°C)
	C_1	C_2	C_3	C_1	C_2	C_3	C_1	C_2	C_3	
P1	2	1	3	0	15	0	100	100	100	40
P2	5	0	15	50	100	30	100	200	250	100
P3	30	4	0	100	100	100	800	750	600	75
P4	4	22	17	400	380	250	800	800	800	50

et al. (2005b) when capital as well as annual operating costs are considered.

6.2. Example 2

The second example (Table 3) is the same as the first one, except that, the contaminant loads are scaled down by a factor of 3.6. As in the previous example, the heat exchanger network was designed to handle fresh water and discharge waste water streams, excluding process to process streams.

The network presented in Fig. 8 is also a feasible solution of example 2, if water flow rates, heat duties, and areas of heat exchange units are scaled down by the same factor used to reduce contaminant loads. The corresponding total area of all the heat exchange units (including the heater) is 1008.5 m^2 and the corresponding capital costs, and annual operating costs would be 0.284 M$ and 2.131 M$/a, respectively. Nevertheless, such a solution is suboptimal.

The optimal network has the same annual operating costs (2.131 M$/a), but lower HEN capital cost (0.281 M$) and is depicted in Fig. 10. The corresponding HEN consists of only two heat exchangers with a total area of 1226.8 m^2, and a single heater (36.7 m^2). The fresh water intake is 90 t/h.

Note that the interconnections between water using process units (water reuse), comparing the solutions presented in Figs. 8 and 10, have not changed due to the contaminant load scale-down. However, the topology of HEN has changed. The reason is that due to the economy of scale, it is more cost effective to have smaller number of heat exchangers with 25% larger area.

We conclude that simultaneous cost-driven synthesis of heat integrated networks is important for obtaining economically attractive solutions and that solutions solely based on minimizing a weighted sum of fresh water consumption and utility usage ignoring capital investment, or sequential procedures are not necessarily the best.

Table 5
Data for example 4 (water using process units)

Process	L^I (kg/h)			c_{max}^{IN}(mg/kg)			c_{max}^{OUT}(mg/kg)			T_p (°C)	
	C_1	C_2	C_3	C_1	C_2	C_3	C_1	C_2	C_3	IN	OUT
P1	6	3	4	5	150	100	50	200	200	25	35
P2	5	8	1	150	120	60	300	150	30	100	85

Table 6
Data for example 4 (regeneration unit)

Regeneration unit	η (%)			T_r (°C)	
	C_1	C_2	C_3	IN	OUT
R	75	90	90	40	37

6.3. Example 3

The third example (Table 4) is an extension of the second example to consider multiple contaminants (three). The number of process units and their operating temperatures are the same as in example 2. Also, the mass load of contaminant C_1, and its inlet–outlet concentration constraints are the same as in example 2.

The solution of example 3 is depicted in Fig. 11. As in example 2, no cooling is needed—the problem is pinched at the fresh water temperature (20 °C). However, the topology of the network differs from the one presented in Fig. 10. First, the presence of additional contaminants altered the interconnections among the water using

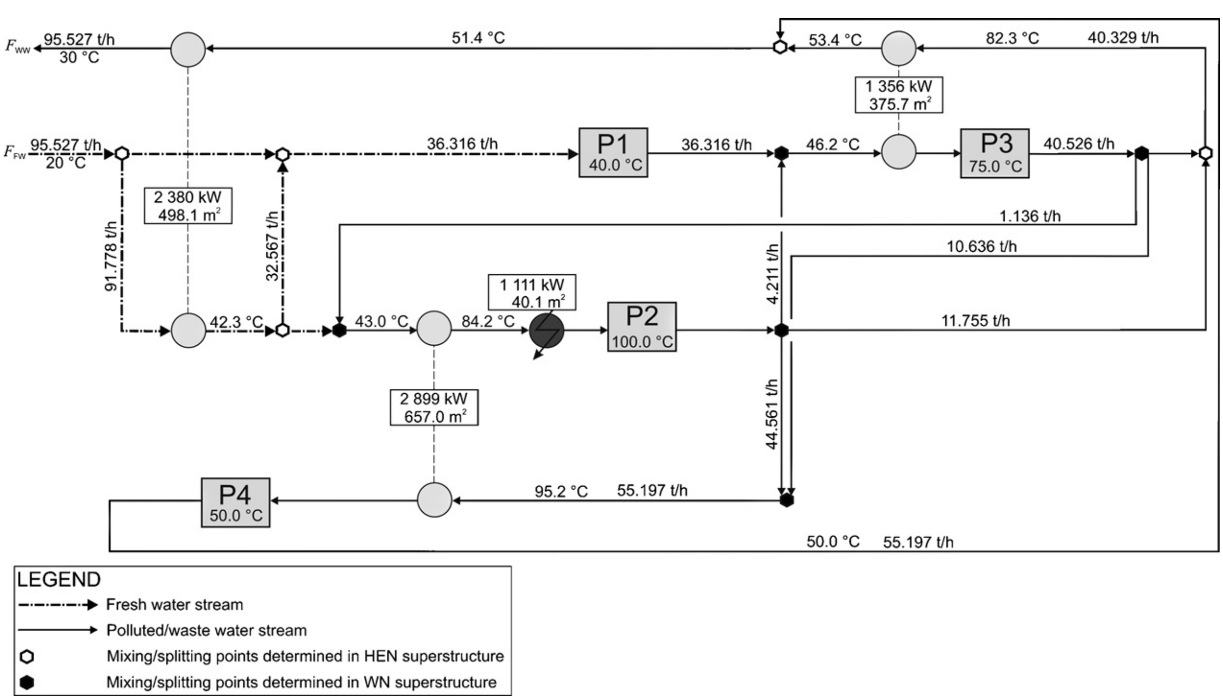

Fig. 11. Solution of multi-contaminant example.

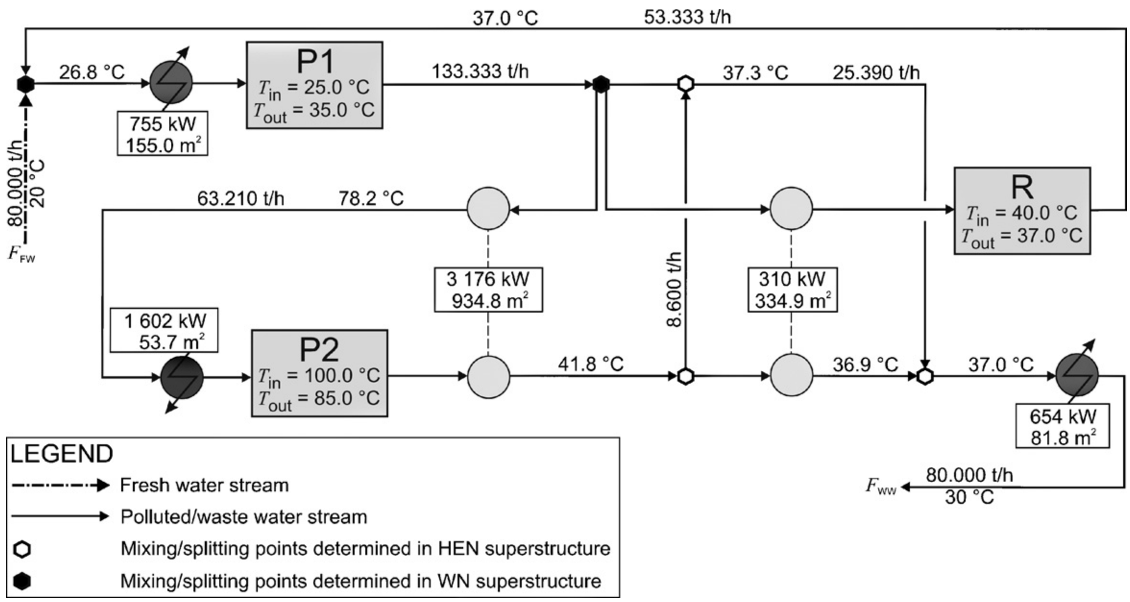

Fig. 12. Solution of multi-contaminant example with regeneration.

Table 7
Summary of results for the four examples

Example	F_{FW} (t/h)	C_{FW} (k\$/a)	C_R (k\$/a)	$C_{R,v}$ (k\$)	C_{HEN} (k\$)[a]	C_{HU} (k\$/a)	C_{CU} (k\$/a)	No. of splits (HEN)
1	324.00	6740.8	–	–	621.7	930.4	–	6
2	90.00	1872.5	–	–	281.4	258.4	–	6
3	95.53	1987.4	–	–	356.4	274.4	–	3
4	80.00	1664.4	421.6	444.7	359.0	395.7	200.8	2

[a] Incl. costs of splits (C_{CON}).

process units. Second, the heat exchangers are placed on streams interconnecting mixer units with process units, as well as on fresh and discharge water streams.

The capital cost of the HEN (which has a total area of 1570.9 m^2) is 0.356 M\$ and the fresh water consumption is 95.53 t/h resulting is an annual operating costs of 2.262 M\$/a.

6.4. *Example 4*

Finally, the fourth example is a small scale multi-contaminant case including the possibility of waste water regeneration. Note that in this example the water using process units and regeneration unit operate non-isothermally. A fixed temperature change, regardless of the water flow rate through the units is assumed. The data for operating conditions of water using process units is given in Table 5. The operating conditions of regeneration unit are presented in Table 6.

The solution of example 4 is presented in Fig. 12. Unlike in the first three examples, heating of 1602 kW and cooling of 1409 kW in total is needed. Heat exchanger network consists of five heat exchange units (one heater, two coolers, and two heat exchangers) with total area of 1560.2 m^2, and capital costs of 0.359 M\$.

The total annual operating cost of the resulting network is 2.683 M\$/a, of which approximately 16% corresponds to costs of water regeneration, 22% to annual utility costs, and 62% to annual fresh water costs. Variable cost associated with regeneration unit capacity is approximately 0.445 M\$.

The results for the four examples presented are summarized in Tables 7 and 8. All four water networks operate at minimal fresh water intake. One explanation for this is that an increase in fresh water intake causes the increase in utility consumption. Also, in all the examples, the contribution of annual fresh water costs outweighs the contributions of other annual and capital costs.

Table 8
Problem sizes and computational time

Example	No. of continuous variables	No. of binary variables	Total CPU time (s)
1	749	115	2.64
2	749	115	2.98
3	1431	249	7.55
4	473	55	3.04

Since the objective in all cases was minimization of annualized costs this outcome is in fact not surprising. This may, however, change when some revenue is associated with the operation of water using process units. In such case, minimal fresh water consumption may not be the optimal one.

7. Conclusions

We presented a mathematical programming model to simultaneously synthesize process water networks and their corresponding HENs. A modified HEN superstructure is proposed to allow non-isothermal stream mixing of process streams. The combined model consists of NLP formulation of WN superstructure and MINLP formulation of embedded HEN superstructure.

Since the majority of equations/constraints in the combined model are non-linear and non-convex more than one optimal solution may exist. For this reason, an efficient initialization is needed to obtain globally or at least very good locally optimal solutions. The solution strategy presented in the paper is efficient enough to overcome the problems associated with initialization. In addition it helps to considerably reduce the sizes of the problems.

Four examples have been presented, clearly showing that the proposed method can be used in synthesis of singe- and multi-contaminant heat integrated water networks. The designs obtained show fairly low topological complexity, which is from industrial application point of view highly desirable.

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