Process-Based Graphical Approach for Simultaneous Targeting and Design of Water Network

Chun Deng and Xiao Feng
Dept. of Chemical Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, P.R. China

Denny Kok Sum Ng and Dominic Chwan Yee Foo
Dept. of Chemical and Environmental Engineering, University of Nottingham Malaysia, 43500 Semenyih, Selangor, Malaysia

DOI 10.1002/aic.12508
Published online February 8, 2011 in Wiley Online Library (wileyonlinelibrary.com).

A new process-based graphical approach (PGA) is presented for the simultaneous targeting and design of water network. The PGA is extended from the limiting water profile which was developed for flow rate targeting for a water network. Via PGA procedure, apart from locating the minimum freshwater and wastewater flow rate targets, the water network that corresponds to the minimum flow rate targets is also synthesized simultaneously. The proposed approach handles both fixed load (including operations with water loss and/or gain) and fixed flow rate problems equally well. In addition, the approach can be used to synthesize direct reuse/recycle, regeneration reuse/recycling, and total water network. Furthermore, the proposed approach is applicable for water network with multiple freshwater sources. Three literature examples are presented to illustrate the proposed approach. © 2011 American Institute of Chemical Engineers *AIChE J,* 57: 3085–3104, 2011
Keywords: water network synthesis, water minimization, pinch analysis, regeneration, total water network, multiple resources

Introduction

In recent years, stringent emission legislation and the increased cost of raw material as well as wastewater treatment have motivated the process and manufacturing industries to emphasis on waste minimization in their daily operations. In particular, water network synthesis has gained good attention in both industrial and research communities. Process integration techniques, such as pinch analysis, are widely accepted as promising tools in synthesizing water network in process and manufacturing industries.

In general, water network synthesis may be classified into two main categories,[1,2] i.e., *fixed contaminant load* (FC) and *fixed flow rate* (FF) problems. In the former, water-using processes (e.g., washing, scrubbing, and extraction) are characterized by mass transfer operations where a fixed amount of contaminant is transferred from the contaminant-rich stream to a contaminant-lean stream, i.e., water, which acts as a mass separating agent. In contrast, water-using processes such as boilers, cooling towers, reactors, etc., are characterized as water sinks/sources that consume/generate a fix amount of water in the FF problem. Hence, the main concern of the latter problem is the water flow rate.

In the seminal study of the FC problem, Wang and Smith[3] presented the *limiting composite curve* to locate the minimum freshwater and wastewater targets. In their later study,[4] the authors extended the previous work[3] to handle cases with water loss and/or gain and suggested the use of local recycling to meet the FF constraints. As shown in Wang and

Correspondence concerning this article should be addressed to X. Feng at xfeng@mail.xjtu.edu.cn.

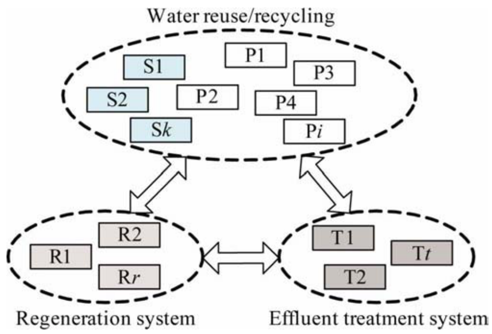

Figure 1. Interactions between individual elements of total water network.

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

Smith,[4] water-using processes which involve water losses/gains are always segregated into two sub-processes; one with uniform inlet and outlet flow rates, and the other with merely flow rate losses/gains. The limiting composite curve that neglects water losses/gains is first plotted. The water supply line is then located by taking into consideration of water losses/gains.[4,5] However, the proposed approaches become cumbersome when it is used for the FF problems that involve many water losses and/or gains. Therefore, in recent years, the development of insight-based targeting tools for the FF problem has been the main focus in the research community.[1,2,6–12] In addition, extension of targeting tools for water network with threshold problems[13] and multiple freshwater resources[14–16] were also reported.

After maximizing water recovery potential via direct reuse/recycle, the freshwater consumption of a water network may be further reduced via regeneration. Wang and Smith[3] extended the use of the limiting composite curve to determine the minimum flow rate targets for regeneration reuse/recycling schemes in the FC problem. In the former scheme, the partially/fully treated water source(s) is restricted to be reused in other processes; while regeneration-recycling scheme allows the treated water to re-enter the process where it is generated. In the previous work,[3] water stream(s) that reach the pinch concentration is selected for regeneration. However, as pointed out by Kuo and Smith,[17] sub-optimum targets may be located when the pinch concentration migrates to a new position after regeneration takes place. Hence, the authors proposed a stream migration procedure[17] to overcome the previous limitation.[3] Although the proposed procedure is useful in determining the minimum water flow rates, the stream migration procedure is iterative in nature and time consuming. In addition, Feng et al.[18] pointed out that the optimal regeneration concentration may not necessarily be located at the pinch concentration. Feng et al.[18] and Bai et al.[19] later presented a revised limiting composite curve[3] to locate the minimum flow rates and the optimal regeneration inlet and outlet concentrations for the water network with regeneration-recycle and regeneration-reuse systems respectively. However, the presented approaches[18,19] are limited to FC problem without water loss or gain. In practice, the FC operations may possess water loss and/or gain which cannot be neglected. Hence, this calls for a revised procedure to overcome the above limitation.

On the other hand, several approaches were developed for water regeneration placement in the FF problems. Hallale[1] first presented guidelines in placing water regeneration units in the water network. As shown in Hallale,[1] the regeneration units are placed across the pinch concentration in order to reduce the overall water flow rates of the network. Later, Manan et al.[2] and Foo et al.[11] based their works on the same principles in synthesizing water regeneration network. However, these works[2,11] are not able to locate the minimum regeneration flow rate. This limitation was later overcome by Agrawal and Shenoy[20] as well as Ng et al.[21]

Conversely, several studies were conducted on the synthesis of distributed effluent treatment network.[22–24] Wang and Smith[22] first proposed the *wastewater treatment composite curve* to target the minimum treatment flow rate for a distributed effluent treatment network. However, the proposed method fails to predict the lowest possible treatment flow rate when multiple treatment units are used. This limitation was then overcome by Kuo and Smith,[23] who proposed an improved targeting procedure. Later, approaches were proposed to identify individual wastewater streams that emit from a water network.[25,26] Besides, targeting approaches were also proposed to determine the minimum treatment flow rate for these wastewater streams.[25–27]

As reported by Kuo and Smith,[24] there are close interactions among the individual elements of a water network, i.e., reuse/recycle, regeneration, and effluent treatment systems. Hence, these systems should be analyzed as a whole in the overall framework known as the *total water network*. Although Kuo and Smith[24] provided the seminal contribution for total water network synthesis, the proposed approach is limited to the FC problem, and is iterative in nature. This limitation is later overcome by the works of Ng et al.[26,27] that synthesize total water network of the FF problem.

Similar to other pinch-based approaches (e.g., heat[28–30] and mass exchange network[31] syntheses), the water network that achieves the flow rate targets is always designed in the second stage once the flow rate targets are located. This can be carried out using the established network design techniques, such as water grid diagram,[3] water main method,[24,29,32] water source diagram[33] for the FC problems; source sink mapping diagram,[31,34] nearest neighbor algorithm,[10,35] and network allocation diagram[12] for the FF problems. Subsequently, a preliminary synthesized network can be improved to reduce its complexity.[36–38] A state-of-the-art review of the various targeting and design techniques for water network synthesis are recently reported by Foo.[39]

Based on above review, it is worth noting that the synthesis of water network based on pinch analysis technique is always carried out in two stages, i.e., targeting and design. The recent review suggested that simultaneous targeting and design for a water network is of good potential for future development.[39] To date, only one study has been reported on this direction.[12] However, the sequential targeting and design steps of this technique that follow the conventional pinch analysis practice has render its extension into a truly simultaneous procedure.[39]

In this article, a new *process-based graphical approach* (PGA) for simultaneous targeting and design of water network is presented. The proposed PGA procedure is developed based on FC problem. However, as point out by the

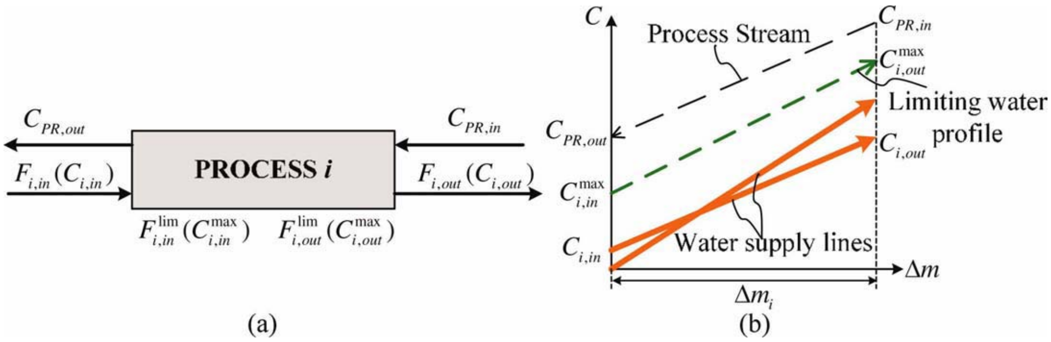

Figure 2. (a) A water-using process; (b) Limiting water profile and water supply lines.[3]

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

recent review,[39] the FC and FF problems for a single contaminant system are equivalent and may be solved by any of the synthesis tools of either groups. Therefore, the proposed PGA is applicable for both FC and FF problems, and can be used to synthesize water networks with direct reuse/recycle and regeneration schemes, as well as total water network. Three literature examples are solved to illustrate the newly proposed approach.

Problem Statement

As shown in Figure 1, a total water network comprises of three water elements, i.e., water reuse/recycle, regeneration and effluent treatment systems. In the water reuse/recycle system, the water-using processes (P1, P2, …, Pi, $i \in \{1, 2, …, N_P\}$) may include FF or FC types (with water loss and/or gain). Note that the FF-types water-using processes are characterized by individual process sinks (inlets) and sources (outlets). External freshwater sources (S1, S2, …, Sk, $k \in \{1, 2, …, N_S\}$) are available to supplement the use of process sources. Effluent from the water-using processes may be sent to regeneration units (R1, R2, …, Rr, $r \in \{1, 2, …, N_R\}$) for further reuse/recycle within the water-using processes or treated in treatment units (T1, T2, …, Tt, $t \in \{1, 2, …, N_T\}$) prior to final environmental discharge. In this work, it is assumed that separate regeneration and wastewater treatment units are employed in the total water network.

The objective of this work is to develop a graphical procedure for the simultaneous targeting and design of a water network that achieves the minimum flow rates targets (freshwater resource(s), regenerated water, and waste treatment), as well as minimum contaminant load removal in the regeneration and treatment units.

Limiting Water Profile and Limiting Composite Curve[3]

In this section, the conventional targeting technique of limiting composite curve[3] is first reviewed. It is then extended to the proposed PGA procedure for simultaneous targeting and design of water network. Figure 2 shows a *limiting water profile* of a water-using process, which is plotted on a concentration vs. mass load diagram known as the *water profile diagram* (WPD). For a given contaminant mass load (Δm_i) to be removed by water, and the given limiting inlet concentration ($C_{i,\text{in}}^{\max}$) of water-using process, the limiting outlet concentration ($C_{i,\text{out}}^{\max}$) is to be maximized to minimize the water flow rate. The minimum limiting water flow rate ($F_{i,\text{in}}^{\lim}$) can be determined via Eq. 1.

$$\Delta m_i = F_{i,\text{in}}^{\lim}(C_{i,\text{out}}^{\max} - C_{i,\text{in}}^{\max}) \tag{1}$$

Since any water supply line that is located below the limiting water profile (with inlet concentration, $C_{i,\text{in}} < C_{i,\text{in}}^{\max}$, and outlet concentration, $C_{i,\text{out}} < C_{i,\text{out}}^{\max}$) can be used to remove the given Δm_i (see Figure 2b). Based on Eq. 1, it is noted that for a given Δm_i, any water flow rate (with inlet concentration of $C_{i,\text{in}}$) can be minimized by maximizing its outlet concentration ($C_{i,\text{out}}$) to the limiting value, i.e., $C_{i,\text{out}}^{\max}$. To determine the minimum flow rate targets for a water network, the limiting composite curve is then plotted by combining the individual limiting water profiles, as shown in Figure 3a. Minimum flow rate of pure freshwater is then targeted by taking the inverse slope of the steepest water supply line that starts at the origin and touches the limiting composite curve, where the *pinch concentration* is formed, as shown in Figure 3b. The latter represents the overall bottleneck for maximum water recovery.

For water-using processes that require uniform flow rate (for most FF problems), local recycling can be used to fulfill the flow rate requirements.[4] On the other hand, for processes with significant water loss/gain, modifications of the previous work[3] are needed to accommodate the water loss/gain. This is the subject of this work. The limiting water profile[3] is further extended to locate water targets for processes with water loss/gain.

Revised Limiting Water Profile

Based on earlier discussion, it is clear that FC problems can be broadly classified into four categories, i.e., processes without water loss/gain, processes with water loss, process with water gain, as well as processes with FF constraints.[4] In this work, the limiting water profiles for processes without water loss/gain,[3] as well as processes with FF constraints[4] remain the same as previous works. In contrast, revised limiting water profiles are introduced for processes with water loss/gain. The revised procedures are described in detail in the following sub-sections.

To address FF processes with water loss/gain, *pseudo-mass load* (the mass load difference between the inlet and outlet of the processes when water loss/gain is being

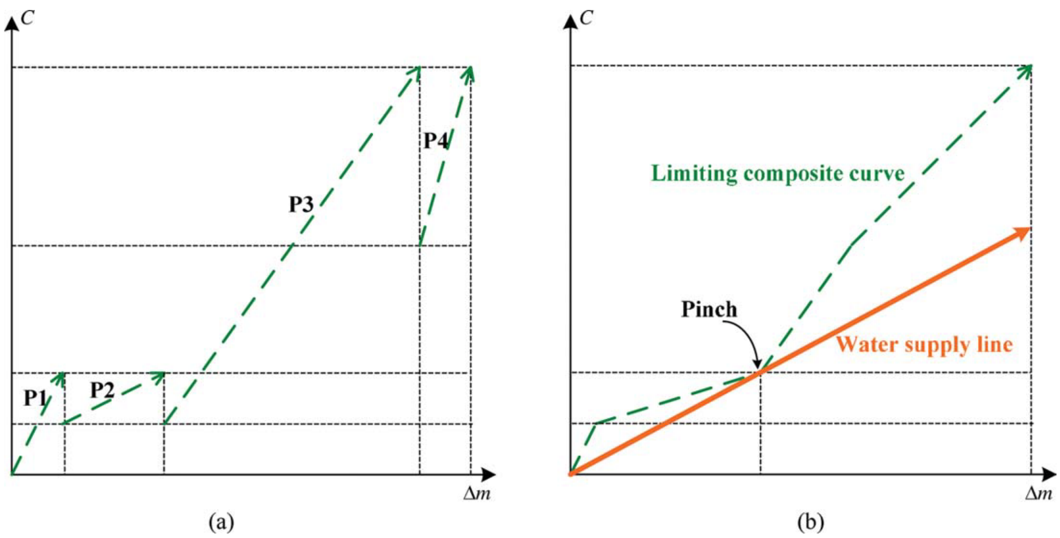

Figure 3. Construction of limiting composite curve from limiting water profiles.[3]

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

ignored) can be determined by Eq. 1. When addition mass load (processes with water gain) or mass load removal (processes with water loss) is involved in such processes, Eq. 1 is revised as below:

$$\Delta m_i^{\text{net}} = F_{i,\text{out}}^{\text{lim}} C_{i,\text{out}}^{\max} - F_{i,\text{in}}^{\text{lim}} C_{i,\text{in}}^{\max} \tag{2}$$

where Δm_i^{net} is termed as *net mass load* difference between outlet and inlet of a water-using process.

Process with water loss

Figure 4a shows a generic model for a water-using process with water loss. Cooling towers with water evaporation loss is a typical example for this type of process. To maintain the cooling water supply, make-up water is needed to supplement the loss. The loss flow rate (F_i^{loss}) is given as the difference between the inlet ($F_{i,\text{in}}$) and outlet ($F_{i,\text{out}}$) flow rates of the process, i.e.:

$$F_i^{\text{loss}} = F_{i,\text{in}} - F_{i,\text{out}} \tag{3}$$

Considering water loss, the mass load difference (Δm_i^{loss}) between the pseudo-mass load and the net mass load of the process is determined by Eq. 4:

$$\Delta m_i^{\text{loss}} = \left|\Delta m_i - \Delta m_i^{\text{net}}\right| = F_i^{\text{loss}} C_{i,\text{out}}^{\max} \tag{4}$$

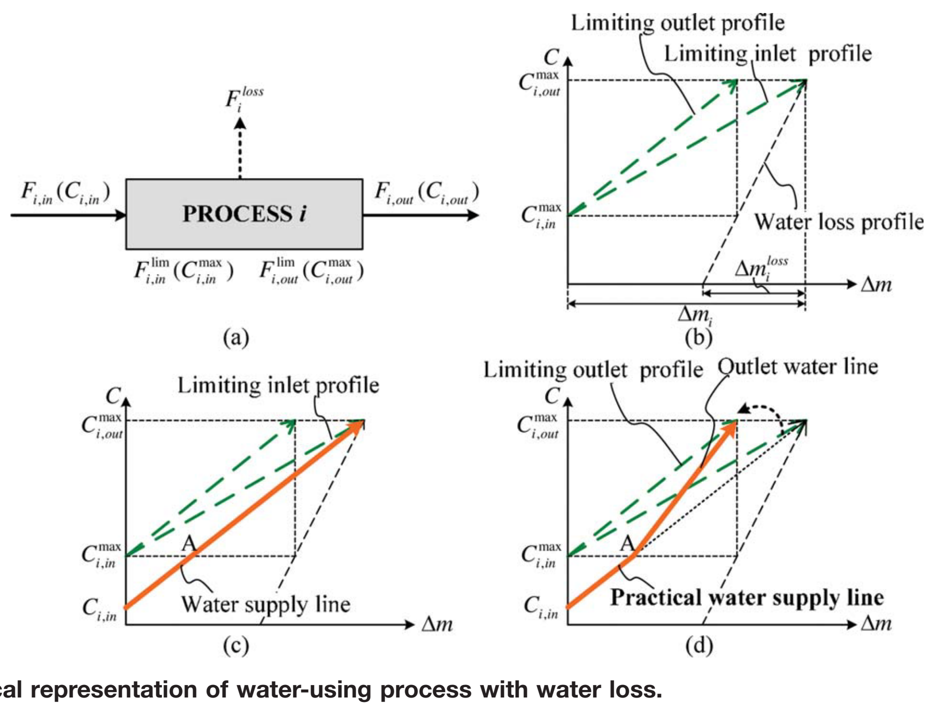

Figure 4. Graphical representation of water-using process with water loss.

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

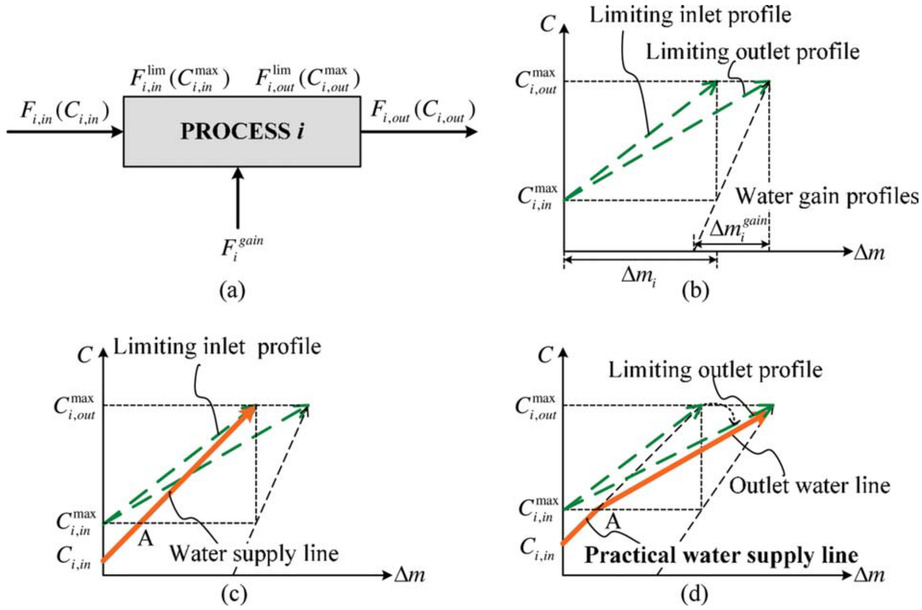

Figure 5. Graphical representation of water-using operation with water gain.

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

To plot a revised limiting water profile for process with water loss, a *limiting inlet profile* is first constructed within the concentration intervals of $C_{i,\text{in}}^{\max}$ and $C_{i,\text{out}}^{\max}$ in the WPD, as shown in Figure 4b. The limiting inlet profile has a horizontal distance of Δm_i, which is determined using Eq. 1. Note also that water loss is not considered at this stage. The inverse slope of limiting inlet profile hence corresponds to the limiting inlet flow rate of the process. Next, *water loss profile* is plotted in the diagram, with its arrow head connected to that of the limiting inlet profile, and with its inverse slope corresponds to F_i^{loss}. In this case, the horizontal distance of the water loss profile indicates the mass load difference for process with water loss, Δm_i^{loss} (calculated using Eq. 4). Next, the *limiting outlet profile* is constructed in the same concentration interval of the limiting inlet profile, with its inverse slope corresponds to the limiting outlet flow rate ($F_{i,\text{out}}^{\text{lim}}$) calculated using Eq. 3.

After the limiting profiles of the water-using process are constructed, the *water supply line* is next located in the WPD. For a water source of concentration $C_{i,\text{in}}$ (lower than $C_{i,\text{in}}^{\max}$), the water supply line is first placed as a straight line between intervals $C_{i,\text{in}}$ and $C_{i,\text{out}}^{\max}$, as shown in Figure 4c. It is then observed in Figure 4c that the water supply line intersects with the $C_{i,\text{in}}^{\max}$ interval line at point A. To determine the *practical water supply line* which considers water loss in the process, the water supply line is rotated anticlockwise at point A until it touches the limiting outlet profile, as shown in Figure 4d. Note that two individual segments are then formed in the practical water supply line. Portion below point A is referred to as the *inlet segment*, while the segment between the $C_{i,\text{in}}^{\max}$ and $C_{i,\text{out}}^{\max}$ interval is the *outlet segment* of the water-using process. Finally, the slope of these respective segments determines the inlet and outlet flow rates of the water-using process.

Process with water gain

Figure 5a shows the generic model for a process with water gain. A good example for this process is water generation as by-product in the reactor. Similar to processes with water loss, a revised limiting water profile is proposed for water-using process with water gain. The water gain flow rate (F_i^{gain}) can be determined by the difference between the inlet and outlet flow rates, as shown in Eq. 5.

$$F_i^{\text{gain}} = F_{i,\text{out}} - F_{i,\text{in}} \tag{5}$$

Considering water gain, the mass load difference (Δm_i^{gain}) between the pseudo-mass load and the net mass load of the process is determined by Eq. 6:

$$\Delta m_i^{\text{gain}} = \left|\Delta m_i - \Delta m_i^{\text{net}}\right| = F_i^{\text{gain}} C_{i,\text{out}}^{\max} \tag{6}$$

In the WPD, the limiting inlet and outlet profiles of the process are first constructed in the $C_{i,\text{in}}^{\max}$ and $C_{i,\text{out}}^{\max}$ intervals (Figure 5b), with their inverse slope corresponds to their respective limiting inlet ($F_{i,\text{in}}^{\text{lim}}$) and outlet ($F_{i,\text{out}}^{\text{lim}}$) flow rates, respectively. Next, the *water gain profile* is added in the diagram, with its arrow head connected to that of the limiting outlet profile, and located within the concentration interval of zero to $C_{i,\text{out}}^{\max}$. The inverse slope of the water gain profile hence corresponds to gained flow rate, F_i^{gain}, while its horizontal distance indicates the mass load difference for process with water gain, Δm_i^{gain} (as shown in Figure 5b) which can be determined via Eq. 6.

For a given water source with an inlet concentration of $C_{i,\text{in}}$ ($\leq C_{i,\text{in}}^{\max}$), the inlet segment of the practical water supply line is initiated at $C_{i,\text{in}}$ and touches the limiting inlet profile at $C_{i,\text{out}}^{\max}$ (see Figure 5c), with its inverse slope corresponds to the supply flow rate. It is then observed in Figure 5c that the water supply line intersects with the $C_{i,\text{in}}^{\max}$ interval line at point A. To determine the practical water supply line which considers water gain in the process, the water supply line is rotated clockwise at point A until it touches the water gain profile, as shown in Figure 5d. Note that two individual segments are then formed in the practical water supply line. Portion below point A is referred as the inlet segment, while that between the $C_{i,\mathrm{in}}^{\max}$ and $C_{i,\mathrm{out}}^{\max}$ interval is the outlet segment of the water-using process. Finally, the slope of these segments determines the respective inlet and outlet flow rates of the water-using process.

Process with multiple feeds

For water-using process with single water source, the supplied water flow rate can be targeted based on the procedure proposed by Wang and Smith.[3] However, such procedure does not cater for cases where multiple water sources are used. Hence, a revised procedure is proposed in this article to cater the latter case.

For a water network, when there are effluents of different impurity concentrations generated from processes (known as *internal water source*), they should be prioritized for reuse/recycle before an external water source is considered. Therefore, it is possible that a water-using process is fed by multiple sources. This is illustrated in Figure 6a. As shown, three sources are available for use in process i, i.e., SR1, SR2, and SR3, each with respective flow rates (F_1, F_2, and F_3) and concentrations (C_1, C_2, and C_3, where $C_1 < C_2 < C_3$). Furthermore, we assume that C_2 has the same concentration as $C_{i,\mathrm{in}}^{\max}$; while C_3 has lower value than $C_{i,\mathrm{out}}^{\max}$. To minimize the cleaner water source (SR1, which is most often an external fresh water source), the reuse of SR2 and SR3 are to be maximized prior to SR1. In this case, SR2 should be fully recovered since $C_2 = C_{i,\mathrm{in}}^{\max}$. In cases where the flow rate of SR2 is insufficient for the process ($F_2 < F_{i,\mathrm{in}}^{\lim}$), the entire flow rate of SR2 (F_2) is used. The removed mass load of SR2, Δm_2 is calculated by Eq. 1. For cases where SR2 has insufficient flow rate, SR3 may also be reused. However, since $C_3 > C_{i,\mathrm{in}}^{\max}$, SR3 needs to be "diluted" with SR1 of lower concentration in order to meet the inlet concentration limit ($C_{i,\mathrm{in}}^{\max}$).

To determine the mixing ratio of SR1 and SR3, the mass and flow rate balances can be solved using Eqs. 7 and 8, respectively. Note that the mass load removed by SR2 (Δm_2) as well as its supplied flow rate (F_2) are to be subtracted from the total requirement of process i (Δm_i).

$$\Delta m_1 + \Delta m_3 = \Delta m_i - \Delta m_2 \tag{7}$$

$$F_1 + F_3 = F_{i,\mathrm{in}}^{\lim} - F_2 \tag{8}$$

where Δm_1 and Δm_3 correspond to the removed mass loads by SR1 and SR3 respectively.

As shown in Figure 6b, water profiles of all sources are constructed within their respective intervals, with a horizontal distance of that corresponds to their mass load removal, as determined by Eqs. 1, 7 and 8. The individual water profiles can then be combined in their respective concentration intervals to form the water supply line, as shown in Figure 6c.

One can analyze the WPD as follows. In concentration interval between the origin and $C_{i,\mathrm{in}}^{\max}(C_2)$, only a single water source SR1 is found (with flow rate F_1). Within concentration interval of C_2 and C_3, the accumulate flow rate of F_1 and F_2 is supplied to the process. Next, in the concentration

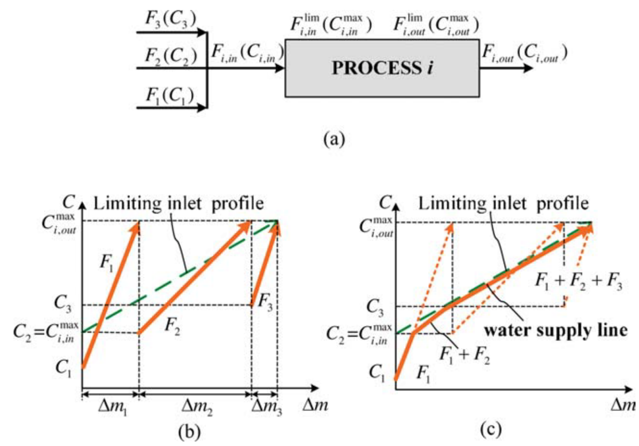

Figure 6. Targeting for water-using process with multiple feeds.

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

interval between C_3 and $C_{i,\mathrm{out}}^{\max}$, the flow rates of SR1, SR2 and SR3 assume to the value of $F_{i,\mathrm{in}}^{\lim}$. Note that the water supply line is identical to limiting inlet profile in the concentration interval above C_3. Note also that the average inlet concentration ($C_{i,\mathrm{in}}$) and inlet flow rate are equal to the maximum inlet concentration ($C_{i,\mathrm{in}}^{\max}$) and limiting inlet flow rate ($F_{i,\mathrm{in}}^{\lim}$), respectively.

It is also worth mentioning a special case for the reuse of SR3 (where $C_3 = C_{i,\mathrm{out}}^{\max}$). In cases where C_3 is equal to the maximum outlet concentration ($C_3 = C_{i,\mathrm{out}}^{\max}$), its corresponding mass load removal (Δm_3) will remain as zero, regardless of its reuse flow rate. Using water source with $C_3 = C_{i,\mathrm{out}}^{\max}$ has the advantage of compensating water flow rate deficit for processes with flow rate loss. The compensating flow rate (F_3) can be determined as $F_{i,\mathrm{in}}^{\lim} - F_1 - F_2$. Note that for this case, the average inlet concentration ($C_{i,\mathrm{in}}$, after source mixing) will then be equal to the maximum inlet concentration ($C_{i,\mathrm{in}}^{\max}$).

Process-Based Graphical Approach (PGA)

In this work, a new PGA procedure is proposed for simultaneous targeting and design for a water network. This approach is an extension of the limiting composite curve of Wang and Smith.[3] As shown previously, the revised limiting water profile for process with water loss/gain is first plotted. Based on the revised limiting water profile, the flow rate allocation for individual process and the associated network design can be determined simultaneously. To illustrate the proposed PGA in detail, three literature examples are solved. In the following section, PGA is applied for the synthesis of reuse/recycle network and water regeneration as well as total water networks.

Example 1—Synthesis of water reuse/recycle network

Table 1 shows the limiting data[4] for a FF problem with five water-using processes with single contaminant constraint. Note that both Reactor and Cooling System streams involve water loss and Filtration stream involves water gain.

Table 1. Limiting Data for Example 1[4]

Operation	Δm_i (kg/h)	$F_{i,\text{in}}^{\text{lim}}$ (t/h)	$F_{i,\text{out}}^{\text{lim}}$ (t/h)	$C_{i,\text{in}}^{\max}$ (ppm)	$C_{i,\text{out}}^{\max}$ (ppm)	Process Sequence P*i*
Reactor	72	80	20	100	1000	5
Cyclone	25	50	50	200	700	4
Filtration	1	10	40	0	100	2
Steam System	0.1	10	10	0	10	1
Cooling System	1.35	15	5	10	100	3
Total	–	165	125	–	–	–

$C_{FW} = 0$ ppm, $C_{R,out} = 200$ ppm, $C_{T,out} = 250$ ppm, $C_{\text{D}}^{\max} = 300$ ppm.

It is assumed that a single pure freshwater supply (0 ppm) is available in service. In this example, a reuse/recycle network with minimum water flow rate targets is first synthesized with PGA. The example is further revisited in later section to illustrate the application of PGA to synthesize water regeneration and total water networks.

Step 1: Preliminary Analysis. First step of the PGA procedure involves the preliminary analysis of the problem. The overall flow rate loss/gain (ΔF_{p}) of the entire water network is first determined via Eq. 9.

$$\Delta F_{\text{P}} = \sum_{i}^{N_{\text{P}}} (F_{i,\text{out}}^{\text{lim}} - F_{i,\text{in}}^{\text{lim}}) \tag{9}$$

A positive value of ΔF_{p} indicates water surplus within the water-using subsystem; while a negative value implies deficit of water. Based on the limiting data in Table 1, ΔF_{p} of Example 1 is determined as – 40 t/h (= 125 t/h – 165 t/h). This indicates that the overall water network experiences a deficit of water flow rate. Hence, freshwater supply of at least 40 t/h is required to supplement the network.

To minimize freshwater consumption, water recovery should be maximized for the internal water sources. To prioritize the use of higher quality (lower concentration) internal water source, the water-using processes are arranged in an ascending order based on their outlet concentrations. For cases where the water-using processes with the same outlet concentrations, such processes are arranged based on their inlet concentrations. Following this procedure, the sequence of the processes in Example 1 is listed in the last column of Table 1. Note that the outlet concentrations of Filtration (P2) and Cooling System (P3) are given as 100 ppm, hence, these processes are arranged based on their inlet concentrations.

For the processes without water loss/gain (i.e., Steam System (P1), Cyclone (P4)), the mass loads are determined with Eq. 1 and shown in the second column of Table 1. For the processes with water loss/gain (i.e., Filtration (P2), Cooling System (P3), Reactor (P5)), the pseudo-mass loads shown in Table 1 are also determined by solving Eq. 1.

Step 2: Targeting and Design. For the water processes without loss/gain, the limiting water profiles are constructed based the procedure proposed by Wang and Smith.[3] However, the limiting water profiles for the processes with loss/gain are constructed based on the newly proposed revised procedure (Figures 4 and 5). Figure 7 shows all the limiting water profiles for all processes in Example 1. Note that the processes are arranged based on the sequence as determined in Step 1 (see Table 1). Filtration (P2) is considered as process with water gain; while Cooling System (P3) and Reactor (P5) are processes with water loss, with their limiting water profiles in Figure 7b, c, and e, respectively.

Since the limiting inlet concentrations of Steam System (P1) and Filtration (P2) are given as 0 ppm (Table 1); only freshwater can be used to fulfill the requirement of these processes. By solving Eq. 1, the minimum freshwater flow rates for P1 and P2 ($F_{\text{FW},1}$ and $F_{\text{FW},2}$) are determined as 10 t/h respectively. As P1 does not involve water loss/gain, the effluent of P1 is determined as 10 t/h with impurity concentration of 10 ppm (see limiting water profile in Figure 7a). Due to 30 t/h of water gain in P2, the outlet flow rate of effluent is determined as 40 t/h at 100 ppm. The revised limiting water profile for P2 is shown in Figure 7b. Effluents from both processes are then taken as internal water sources for other processes, before freshwater is considered.

As shown in Table 1, the limiting inlet concentration of Cooling System (P3) is given as 10 ppm. Hence, 10 t/h of internal water source from P1 (10 ppm) can be directly reused in P3. Solving Eq. 1 determines that a total mass load of 0.9 kg/h is removed by internal water source from P1. Next, freshwater and internal water source at 100 ppm are available for reuse. However, as mentioned previously, since the internal water source has a concentration that is equal to the limiting outlet concentration of P3, i.e., 100 ppm, this water source will not remove any mass load and can only be used for meeting the FF constraint of P3. Thus, the remaining of the 1.35 kg/s mass load of P3, i.e., 0.45 kg/h (= 1.35 kg/h − 0.9 kg/h) is to be removed by freshwater. Based on Eq. 1, the freshwater flow rate is determined as 4.5 t/h. To construct the water supply line in the WPD (Figure 7c), the internal water source segment (10 t/h) is first constructed in the concentration interval between 10 ppm to 100 ppm, and touches at the arrowhead of the inlet profile. Next, 4.5 t/h of freshwater is constructed in the concentration interval between 0 and 100 ppm to the left of the internal water source segment (see Figure 7c). As shown in Figure 7c, the water supply line in concentration interval between 10 ppm and 100 ppm is constructed by combining water supply lines for two sources. Since Cooling System is considered as a FF process, where 15 t/h of water flow rate is required, additional water flow rate of 0.5 t/h (= 15 t/h − 10 t/h − 4.5 t/h) of this process may be supplied either by the internal source from P2 (available at 40 t/h, 100 ppm) or the effluent of P3 via local recycling scheme.[4] The former scheme is recommended, as to avoid the building up of unexpected contaminants within P3 via local recycling. Hence, the remaining internal water source from P2 at 100 ppm is reduced from 40 t/h to 39.5 t/h. The water allocation of P3 is showed in Figure 7f. Note that three water sources are supplied to P3 with an average inlet concentration of 10 ppm. Due to 10

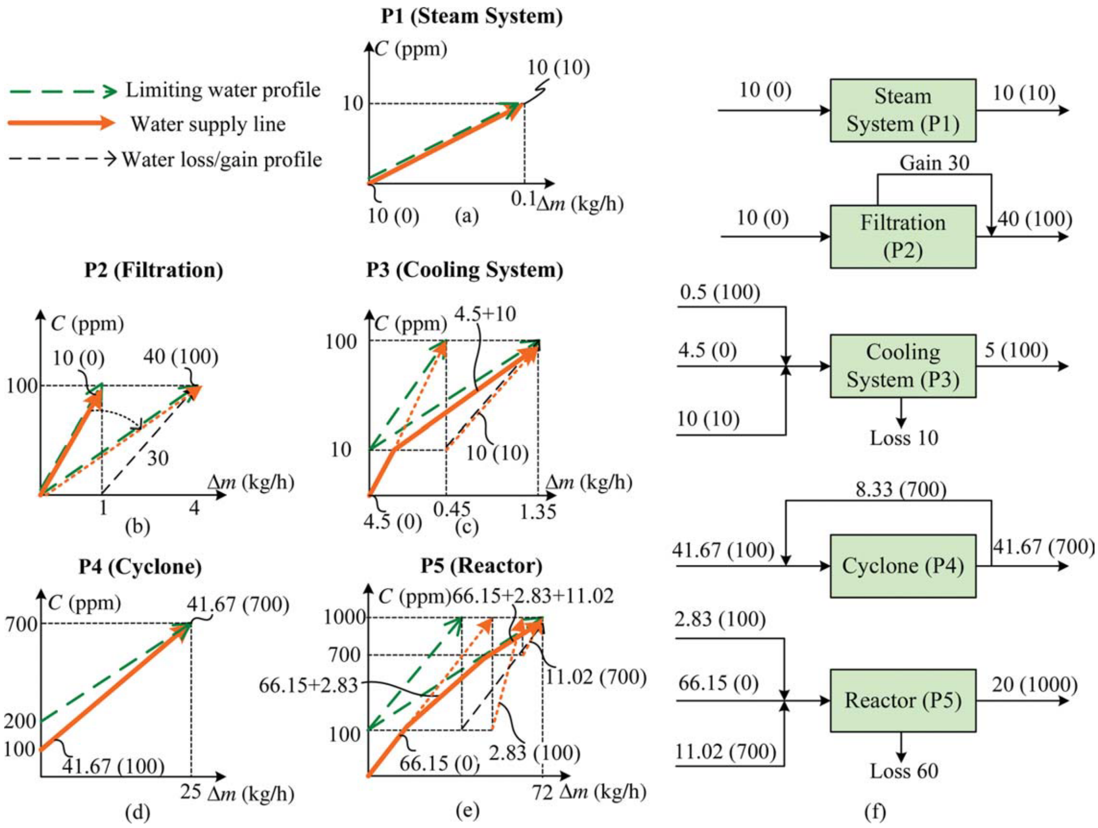

Figure 7. (a)–(e)Targeting for water-using processes P1–P5; (f) Water sources allocation for each water-using process involving flow rate constraints (unit for the flow rate is ton/h and unit for contaminant concentration is ppm in parenthesis).

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

t/h of water loss occurs in this process, the effluent of P3 with 100 ppm is reduced from 15 t/h to 5 t/h. Combining the effluent of P3 with the effluent from P2, the internal water source of 100 ppm is increased from 39.5 t/h to 44.5 t/h.

Next, water allocation for Cyclone (P4) is analyzed. Since a total of 44.5 t/h of 100 ppm internal water source is available, this internal water source should be reused for P4, before the freshwater source is considered. To fulfill the requirement of P4, the flow rate of this internal water source is determined as 41.67 t/h using Eq. 1. Since there is no water gain and loss in P4, the effluent from P4 has the same flow rate as its inlet stream (i.e., 41.67 t/h), with an outlet concentration of 700 ppm (see Figure 6d). To maintain the flow rate requirement for P4 (50 t/h), local recycling scheme[4] is implemented. As shown in Figure 7f, 8.33 t/h (= 50 t/h − 41.67 t/h) of effluent from P4 is being recycled, apart from the reuse of 41.67 t/h of internal water source at 100 ppm. The average inlet concentration is calculated as 200 ppm, which matches the limiting inlet concentration of P4.

After water allocation is completed for P4, two internal water sources are available for Reactor (P5), i.e., effluents from P3 (2.83 t/h = 44.5 t/h − 41.67 t/h, 100 ppm) and P4 (41.67 t/h, 700 ppm), respectively. Since the inlet concentration of P5 is given as 100 ppm, internal water source of 100 ppm can be completely reused in P5. As mentioned previously, if internal water source at 700 ppm is reused, freshwater is required for dilution. Solving mass and flow rate balance Eqs. 7 and 8, 11.02 t/h of internal water source at 700 ppm and 66.15 t/h of freshwater are required to fulfill the process requirement. As shown in Figure 7e, 11.02 t/h of internal water source at 700 ppm is first constructed in the concentration interval between 700 ppm and 1000 ppm. Next, 2.83 t/h of the 100 ppm internal water source is constructed in the concentration interval between 100 and 1000 ppm on the left of the 700 ppm internal water source. Finally, 66.15 t/h of freshwater is plotted in the concentration interval between 0 ppm and 1000 ppm on the left of the 100 ppm internal water source (see Figure 7e). Note that the average inlet concentration and total flow rate are determined as 100 ppm and 80 t/h, which are equal to the limiting inlet concentration and limiting inlet flow rate of P5 (see Table 1). However, due to 60 t/h of water loss, the flow rate of P5 effluent is reduced to 20 t/h.

Based on the detailed allocation of freshwater and internal water sources as shown in Figure 7f, an overall minimum freshwater flow rate is determined as 90.65 t/h (10 t/h, 10 t/h, 4.5 t/h and 66.15 t/h for P1, P2, P3 and P5, respectively); while the overall wastewater flow rate is determined as 50.65 t/h (30.65 t/h WW1 at 700 ppm, and 20 t/h WW2 at 1000 ppm). Note that both freshwater and wastewater flow rate targets are identical with the earlier reported results.[4,5,40]

It is also worth noting that the individual limiting water profiles in Figure 7 can be combined to plot the limiting

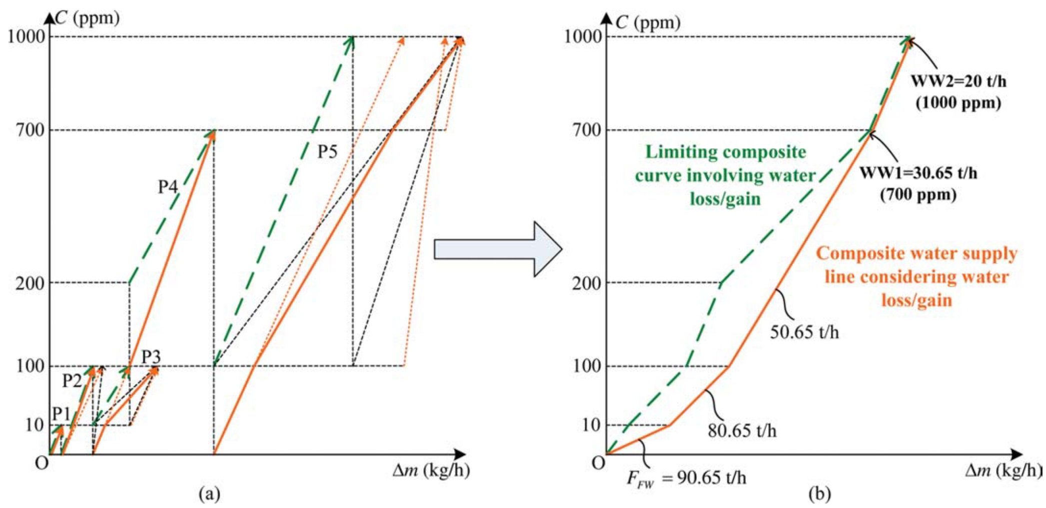

Figure 8. (a) Individual limiting water profiles and water supply lines for all water-using processes; (b) Limiting composite curve and composite water supply line for Example 1 with reuse/recycling.

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

composite curve, as shown in Figure 8a. A revised limiting composite curve (Figure 8b) that considers water loss/gain can then be constructed by combining all individual limiting water profiles in Figure 8a. Note that for the processes with water loss (P3—Cooling System; and P5—Reactor), their limiting outlet profiles are combined into the limiting composite curve. The underlying principle is that, the water loss is assumed to happen in the inlet of the process. In contrast, for the process with water gain (P2—Filtration), its limiting outlet profile is excluded in the construction of the limiting composite curve (only its limiting inlet profile is included). In other words, the model assumes that water gain is found at the outlet of the process.

Besides, the corresponding *composite water supply line* can be determined by combining the water supply lines for all processes within the respective concentration intervals, similar to the construction of the limiting composite curve. Note that this composite water supply line takes into account the water loss/gain of the individual process. As shown in Figure 8b, the total flow rates found between 0 ppm and 10 ppm corresponds to the overall freshwater flow rate (F_{FW}) of 90.65 t/h. The summation of the flow rates in the next concentration interval (10 ppm to 100 ppm) gives 90.65 t/h. However, due to 10 t/h of water loss (in Cooling System) at 10 ppm, the flow rate of water supply is reduced to 80.65 t/h. It is noted that the slope of the composite water supply curve in concentration interval between 10 ppm and 100 ppm increases slightly when compared with previous concentration interval. For concentration interval between 100 ppm and 700 ppm, the total flow rates is calculated as 110.65 t/h (= 41.67 t/h + 66.15 t/h + 2.83 t/h). In this concentration interval, 30 t/h of water gain (Filtration) occurred at 100 ppm, which increases the water supply flow rate from 80.65 t/h to 110.65 t/h. On the other hand, 60 t/h of water loss (Reactor) also occurred, thus, the practical water supply flow rate reduced to 50.65 t/h (= 110.65 t/h − 60 t/h). The summation of water supply flow rates in the final concentration interval (700 ppm − 1000 ppm) gives 80 t/h (= 66.15 t/h + 2.83 t/h + 11.02 t/h). Because of 60 t/h of water loss in Reactor, the practical water supply flow rate in this interval is reduced to 20 t/h (= 80 t/h − 60 t/h). Since 50.65 t/h of internal water source generated from previous concentration

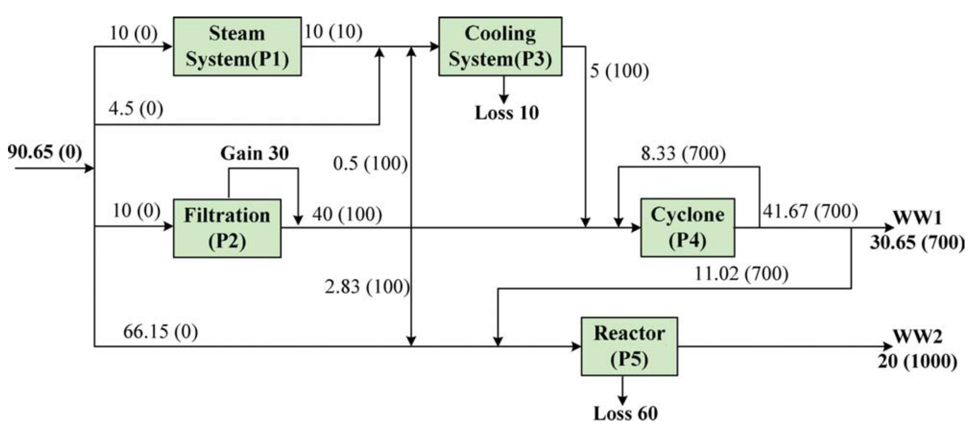

Figure 9. An optimal water network for Example 1 with reuse/recycling.

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

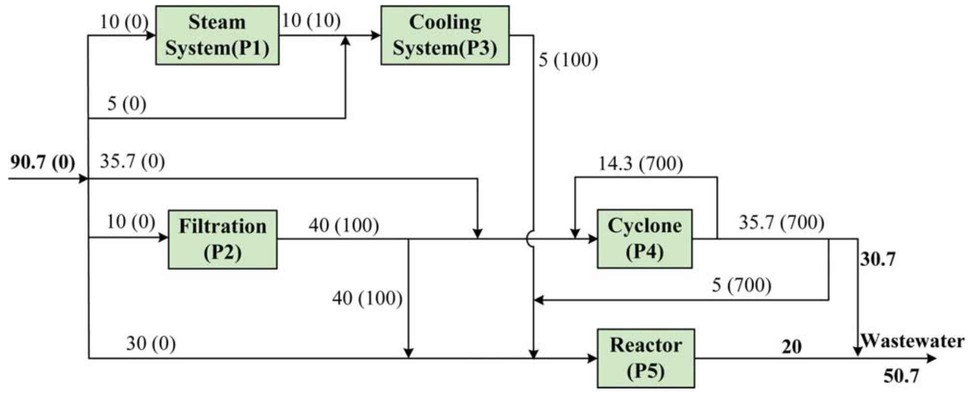

Figure 10. Water network for Example 1 reported by Wang and Smith.[4]

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

interval at 700 ppm, a surplus of 30.65 t/h (= 50.65 t/h − 20 t/h) of internal water source is discharged as wastewater (denoted as WW1). Besides, 20 t/h of wastewater (WW2) is generated at 1000 ppm, from the last concentration interval. Note that the corresponding flow rate of each concentration interval can also be determined based on the inverse slope of each segment of the composite water supply line in the respective concentration interval (Figure 8).

Combining all the individual networks in Figure 7f, a final water network design for direct reuse/recycle scheme was constructed, as shown in Figure 9. Note that the network design in Figure 9 is slightly different as compare with those reported in the literature.[4,5,40] Figures 10–12 show several alternative designs reported by Wang and Smith,[4] Mann and Liu,[5] and Jeżowski et al.,[40] respectively. Note that all alternative designs have quite similar stucture. As compared with Figure 10, the local recycle stream of Cyclone (P4) in Figure 9 has a lower flow rate (8.33 t/h, when compared with 14.3 t/h in Figure 10). Besides, higher flow rate of freshwater (66.15 t/h) is being allocated to Reactor (P5) in Figure 9 (when compared with 30 t/h in Figure 10). Both of these flow rate allocations reduce the buildup of unexpected contaminant within P4 and P5 (when compared with that in Figure 10). On the other hand, the blow down of Cooling System (P3) may be contaminated with treatment chemicals, hence it is not advisable to reuse the blow down to reactor which would be sensitive to the contamination (as shown in Figure 10). Therefore, to reduce the risk, a penalty of 5 t/h in freshwater is suggested, which increases the freshwater flow rate unnecessarily.[4] However, as shown in Figure 9, water from Cooling System (P3) is not reused in Reactor (P5); thus, no penalty of freshwater is required.

Besides, comparison may be made for the network design in Figure 9 and Figure 11. As shown in Figure 9, the additional 0.5 t/h internal water source is allocated to the Cooling System (P3) from Filtration (P2) to maintain the FF requirement of the former. Besides, similar to the design in Figure 10, the higher flow rate of local recycle stream for Cyclone (P4; 14.29 t/h), and lower freshwater flow rate to the Reactor (P5; 30.43 t/h) make the design in Figure 11 having higher tendency of trapping unexpected contaminants in those units, when compared with the design in Figure 9.

Finally, in Figure 12, the interconnections with water flow rates lower than 2 t/h have been eliminated. Hence, the freshwater consumption is slightly higher for the network in Figure 12, when compared with that in Figure 9. However, it is worth mentioning that the internal water source from Cooling System is not directed to the Reactor (P5), as in the case of Figures 10 and 11. Besides, lower local recycle flow rate for Cyclone (P4; 8.36 t/h), and higher freshwater flow rate to the Reactor (P5; 65.69 t/h) make the design in Figure 12 to have the advantage of trapping less unexpected contaminants in those units, similar to the design in Figure 9.

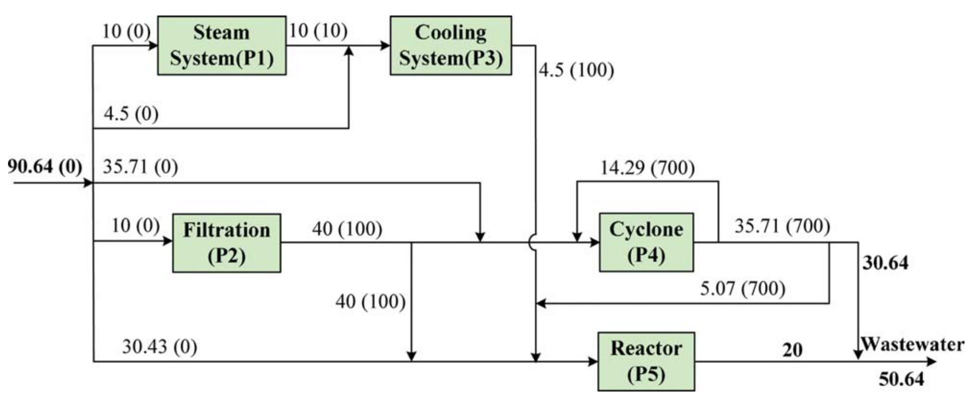

Figure 11. Water network for Example 1 reported by Mann and Liu.[5]

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

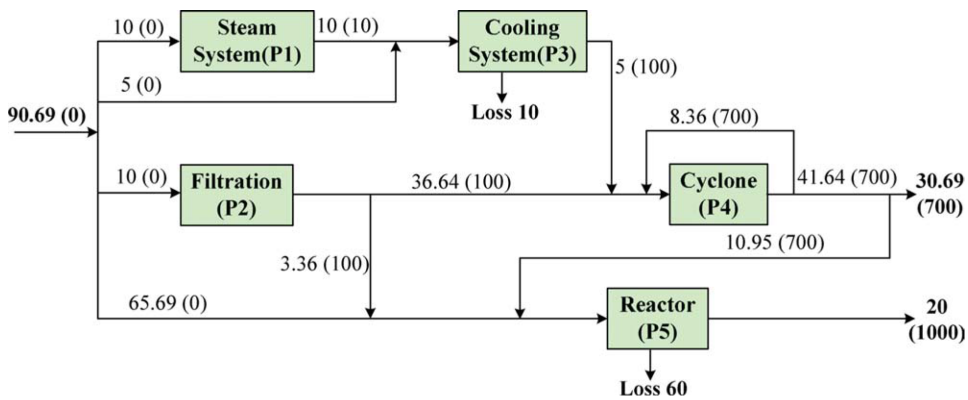

Figure 12. Water network for Example 1 reported by Jeżowski et al.[40]

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

Synthesis of water network with regeneration unit

After the maximum water recovery potential is exhausted via reuse/recycle scheme, freshwater consumption can be further reduced by partial treating the process effluent (often known as *regeneration*) for further recovery. According to Wang and Smith,[3] regeneration processes may be broadly classified as fixed outlet concentration ($C_{\mathrm{R,out}}$) and fixed removal ratio (RR). For the former, the performance is rated based on the postregeneration concentration of the regeneration unit ($C_{\mathrm{R,out}}$);[18,19,21,41] while regeneration unit of RR type is rated based on fraction of mass load removal from the water streams.

In this study, only regeneration unit of the fixed $C_{\mathrm{R,out}}$ type is taken into consideration. The regenerated water can be treated as a new water source to fulfill the requirement of the water sinks. Example 1 is revisited to illustrate the proposed approach for water network with regeneration.

Example 1 (revisited)

Steps 1 and 2: In this example, the $C_{\mathrm{R,out}}$ value is set as 200 ppm. For this case, Step 1 (preliminary analysis) that was proposed for reuse/recycle scheme remains the same. In contrast, Step 2 (targeting and design) is modified slightly in this case as additional water source from regeneration is available. In addition, selection of streams for regeneration is to be determined by the PGA procedure.

Following the previous proposed approach, the limiting water profiles for all processes are first constructed. The allocation of water source for each process is performed based on the sequence that identified in Step 1. Note that since the regenerated water has an outlet concentration of 200 ppm, thus, it will only be needed when the internal water sources of lower concentration are exhausted. Note also that P1, P2, and P3 have limiting outlet concentrations that are lower than $C_{\mathrm{R,out}}$ (200 ppm), thus, the regenerated water cannot be used in these processes (or else higher freshwater flow rate is required for dilution). Therefore, the water allocation schemes for P1–P3 are identical to the reuse/recycle scheme, as shown in Figure 7a–c.

Since P4 and P5 may accept regenerated water to reduce freshwater consumption, the detailed procedure for P4 and P5 is shown in Figure 13. Note that from the reuse/recycle scheme, it is observed that 44.5 t/h of effluent at 100 ppm is generated from P2 and P3 (see Figure 7), which may be used as internal source for water recovery apart from the regenerated source. To minimize the usage of this higher quality source and freshwater, the 100 ppm source will only

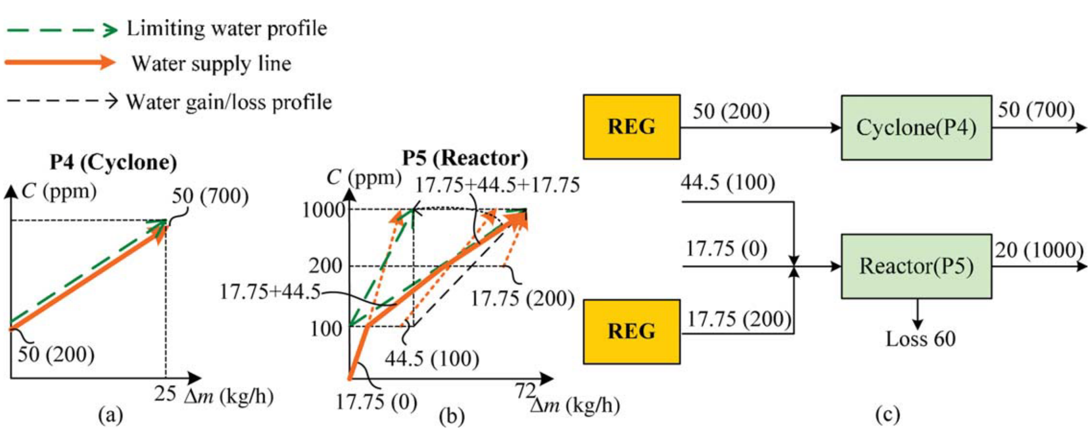

Figure 13. (a)–(b)Targeting for processes 4 and 5 involving regeneration process; (c) Water sources allocation for processes 4 and 5 with flow rate constraints involving regeneration process.

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

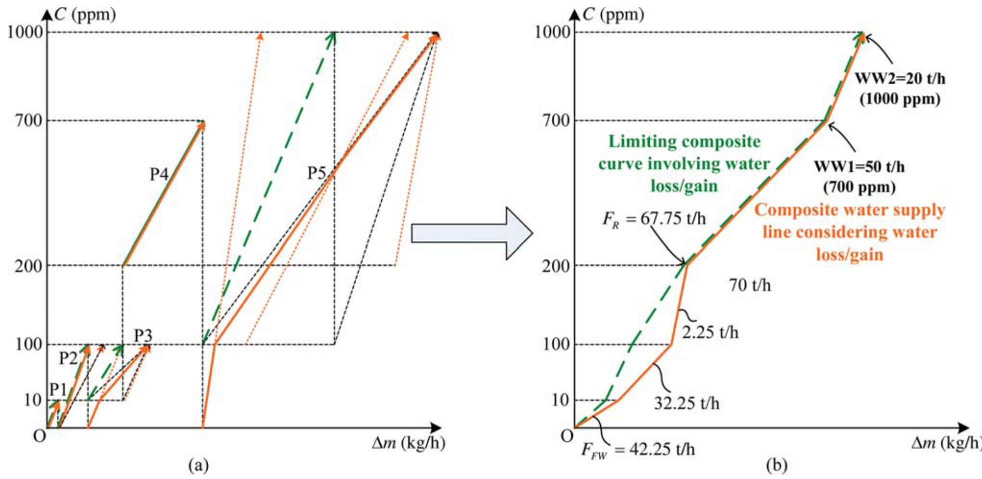

Figure 14. (a) Individual limiting water profiles and water supply lines for all water-using processes; (b) Limiting composite curve and composite water supply line for Example 1 with regeneration reuse/recycle.

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

be used when both internal water and regenerated sources of lower quality are exhausted. Since the regenerated water of 200 ppm has the same concentration as $C_{i,\text{in}}^{\max}$ of P4, it is first selected for recovery; with its flow rate determined as 50 t/h based on Eq. 1. Note that there is no water loss/gain in P4, thus, both inlet and outlet flow rates remain constant (50 t/h) with an outlet concentration of 700 ppm. This is represented in Figure 13a where the water supply line overlaps with the limiting water profile.

On the other hand, four water sources are available for P5, i.e., freshwater, regenerated water of 200 ppm and internal water sources of 100 ppm and 700 ppm. Since the internal water source of 100 ppm has the same concentration as $C_{i,\text{in}}^{\max}$ of P5, it is first selected for recovery. Next, we should determine if P5 is to be fed with regenerated water (200 ppm) or the leftover internal water source (700 ppm). Since both water sources have concentration higher than the limiting inlet concentration of P5 (100 ppm), freshwater is needed for dilution. Since the regenerated source is of lower concentration, it requires less freshwater for dilution. Thus, freshwater (0 ppm) and regenerated water (200 ppm) are mixed to fulfill the process requirement of 35.5 t/h (= 80 t/h − 44.5 t/h). Using Eqs. 7 and 8, the freshwater ($F_{\text{FW},5}$) and regenerated ($F_{\text{R},5}$) flow rates for P5 are determined as 17.75 t/h respectively. As shown in Figure 13b, three water supply lines for freshwater, regenerated water and internal water source at 100 ppm are plotted in the WPD. Note that the average inlet concentration of 100 ppm is achieved. Meanwhile, the effluent flow rate from P5 is determined as 20 t/h, as 60 t/h of water loss is encountered in this process.

The detailed allocation of freshwater and internal water sources for P4 and P5 is shown in Figure 13c. The minimum flow rates of freshwater, regenerated water and wastewater are determined as 42.25 t/h, 67.75 t/h, and 70 t/h, respectively. Because of all other internal water sources being exhausted, the residual internal water sources are identified as wastewater streams. Hence, two wastewater streams are located at 700 ppm (50 t/h, WW1) and 1000 ppm (20 t/h, WW2),

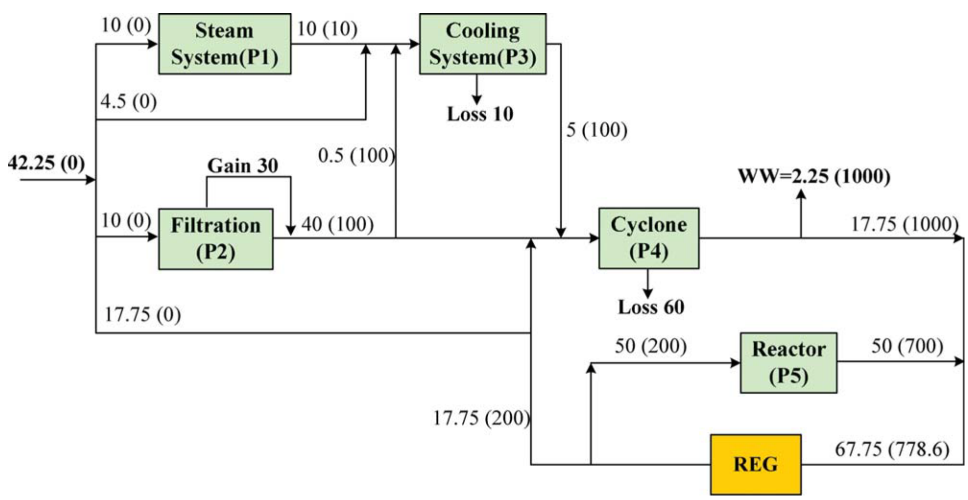

Figure 15. An optimal water network for Example 1 with regeneration process.

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

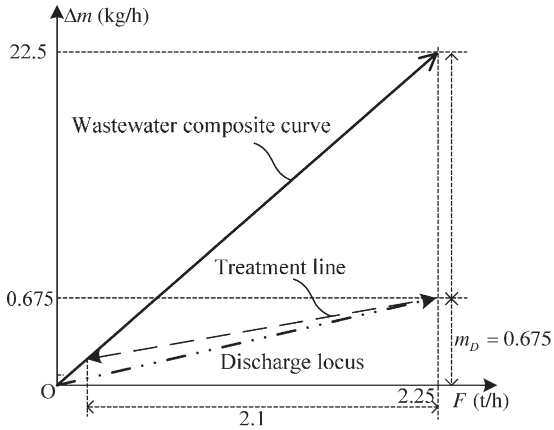

Figure 16. The minimum treatment flow rate targeting for Example 1.

respectively. To fulfill the water requirement of regeneration process, 67.75 t/h of wastewater needs to be regenerated. The selection strategy for wastewater streams that are sent for regeneration will be explained in the following section.

Similar to the direct reuse/recycle scheme, the individual limiting water profiles in Figure 13 are combined in a WPD as shown in Figure 14a. A revised limiting composite curve (Figure 14b) that considers water loss/gain can then be constructed. The corresponding composite water supply line can be determined by combining the water supply lines for all processes with the consideration of water loss/gain. The targeted minimum freshwater flow rate 42.25 t/h and regenerated water flow rate 67.75 t/h are marked on the composite water supply line. Note that the regenerated water is added into the system at 200 ppm, which leads to an increase of slope for the segment on the composite water supply line.

Step 3: Targeting for Minimum Mass Load for Regeneration Process. The mass load removal (Δm_R) for a fixed concentration type regeneration unit can be determined by Eq. 10:

$$\Delta m_R = F_R(C_{R,in} - C_{R,out}) \tag{10}$$

where F_R refers to the regeneration flow rate without considering water loss; $C_{R,in}$ and $C_{R,out}$ denote the pre- and postregeneration concentrations of the regeneration unit, respectively. Based on Eq. 10, it is noted that the regeneration mass load (Δm_R) is a function of $C_{R,in}$, for the given F_R and $C_{R,out}$ values. To minimize the mass load removal in a regeneration unit (hence a small unit), lower concentration stream(s) should be selected for regeneration.[27]

In this example, $C_{R,out}$ is taken as 200 ppm, and the minimum regenerated flow rate (F_R) is targeted as 67.75 t/h in previous step. Earlier step also determines that two wastewater streams are generated from the network, i.e., WW1 (50 t/h, 700 ppm) and WW2 (20 t/h, 1000 ppm). To fulfill the regeneration mass load, the lower concentration WW1 (50 t/h, 700 ppm) is fully regenerated; while the remaining regeneration flow rate requirement (17.75 t/h) is take from WW2 (1000 ppm). The mean inlet concentration of the combined waste stream for regeneration is determined as 778.6 ppm ($C_{R,in}$). Eq. 10 determines the minimum mass load removal as 39.2 kg/h. Similar to the direct reuse/recycle scheme, combining the individual networks in Figure 13c yields a water regeneration network that achieves the minimum water flow rate targets, as shown in Figure 15. The incorporation of regeneration process reduces the freshwater consumption of the water network significantly.

Total water network synthesis

To comply with the environment legislation, treatment units are used to purify the wastewater streams before they are discharged to the environment. Similar to the case of regeneration, waste treatment units may also be categorized into fixed outlet concentration and load RR types.[3,22,23] Kuo and Smith[17] highlighted the similarities between water regeneration and final effluent treatment. When water of better quality is needed for the purpose of reuse/recycle, effluent may be partially or fully regenerated. When the effluent has become too contaminated for reuse/recycle, and/or when the regenerated water can no longer be reused/recycled (e.g., due to the water network has reached its maximum extent of using regenerated water of a given quality), it must be treated before it can be discharged to the environment, to fulfill the environmental discharge requirement.[24]

In this study, a single treatment system of fixed outlet concentration is considered. Wastewater composite curve proposed by Ng et al.[27] is used to locate the minimum

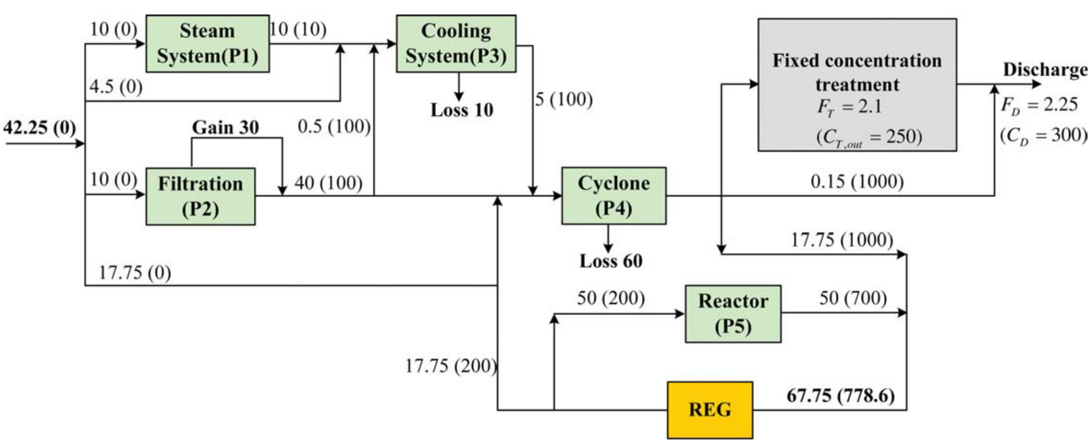

Figure 17. An optimal total water network for Example 1.

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

Table 2. Summary of the Targeting Results for Different Schemes (Example 1)

Schemes	Freshwater Flow Rate F_{FW} (t/h)	Regenerated Water Flow Rate F_R (t/h)	Minimum Treatment Flow Rate F_T (t/h)	Waste Stream	Contaminant Mass Load (kg/h) Freshwater m_{FW}	Water-Using Processes Δm_p	Regeneration Unit Δm_R	Treatment Unit Δm_T	Wastewater Discharge m_D
Reuse/recycle	90.65	–	–	WW1 (30.65 t/h, 700 ppm) WW2 (20 t/h, 1000 ppm)	0	41.45	–	–	41.45
Regeneration Reuse/recycle	42.25	67.75	–	WW (2.25 t/h, 1000 ppm)	0	41.45	39.2	–	2.25
Total water network	42.25	67.75	2.1	WW (2.25 t/h, 300 ppm)	0	41.45	39.2	1.575	0.675

contaminant mass load removal in waste treatment system when necessary. In the previous study,[27] the minimum treatment flow rate is targeted prior the detailed design.

Similar to Eq. 10, the mass load difference (Δm_T) between the inlet ($C_{T,in}$) and outlet ($C_{T,out}$) for a treatment system with fixed outlet concentration model can be determined via Eq. 11 that follows:

$$\Delta m_T = F_T(C_{T,in} - C_{T,out}) \tag{11}$$

where F_T refers to the treatment flow rate without water loss. To determine the minimum treatment mass load Δm_T, the overall mass load balance for the total water network is given in Eq. 12:

$$m_{FW} + \Delta m_P = \Delta m_R + \Delta m_T + m_D \tag{12}$$

where m_{FW}, Δm_p, and m_D denote total mass load of freshwater, overall mass load for all water-using processes, and mass load that is discharged along with wastewater streams from the water network. Those three terms are described in details as follows.

The total mass load of freshwater (m_{FW}) is determined via equation below,

$$m_{FW} = \sum_{k}^{N_S} F_{FW(k)} C_{FW(k)} \tag{13}$$

where $F_{FW(k)}$ and $C_{FW(k)}$ refer as the flow rate and concentration of kth external water source. Note that, if a pure external water source is used, no mass load will be contributed to the water network. In contrast, impure fresh source will contribute additional mass load to the water network.

In addition, the overall mass load balance for water-using subsystem is given as follows,

$$\Delta m_P = \sum_{i}^{N_P} \Delta m_i^{net} = \sum_{i}^{N_P} (F_{i,out}^{lim} C_{i,out}^{max} - F_{i,in}^{lim} C_{i,in}^{max}) \tag{14}$$

In cases where Δm_p takes a positive value, there is surplus of mass load generated from the water-using subsystem. In contrast, a negative value of Δm_p indicates that the water-using subsystem accepts all mass load generated from all process sources and additional mass load from external freshwater without treatment/regeneration.

Meanwhile, m_D can be determined via equation below,

$$m_D = F_D C_D \tag{15}$$

where F_D and C_D are the flow rate and discharge concentration of wastewater. To fulfill the environment legislation, the mean concentration of the wastewater discharge can not exceed the maximum allowable discharge concentration (C_D^{max}). Note that all wastewater streams that are treated or bypass the treatment system are mixed before being discharged to the environment. For cases where there are more than one wastewater stream, the total flow rate of wastewater streams (F_D) is given by Eq. 16.

$$F_D = \sum_{w} F_{WW(w)}^{D} \tag{16}$$

where $F_{WW(w)}^{D}$ denotes the flow rate for wth wastewater streams sent for treatment/discharge.

Example 1 (revisited)

For Example 1, freshwater with 0 ppm is in used; thus, no additional mass load is contributed from freshwater (m_{FW} = 0). Based on the given limiting data in Table 1, Δm_p is determined as 41.45 kg/h by solving Eq. 14. Meanwhile, 2.25 t/h of wastewater is discharged from the water network and F_D is determined as 2.25 t/h based on Eq. 16. Since the maximum allowable discharge concentration (C_D^{max}) is given as 300 ppm, the maximum value of m_D is determined as 0.675 kg/h with Eq. 15. Solving Eq. 12, the minimum treatment mass load (Δm_T) is calculated as 1.575 kg/h. Since there is single wastewater stream, the inlet treatment concentration is 1000 ppm ($C_{T,in}$) and it is treated to 250 ppm ($C_{T,out}$). The minimum treatment flow rate is then determined as 2.1 t/h using Eq. 11. Note that, the same result can be verified by the graphical method proposed by Ng et al.[27] (Figure 16). Figure 17 shows the total water network design for Example 1. As shown, a big portion of the wastewater stream (2.1 t/h) is purified in the treatment process to a reduced concentration

Table 3. Limiting Data for Example 2[3]

Process	Δm_i (kg/h)	$F_{i,in}^{lim}$ (t/h)	$C_{i,in}^{max}$ (ppm)	$C_{i,out}^{max}$ (ppm)	Process Sequence i
1	2	20	0	100	1
2	5	100	50	100	2
3	30	40	50	800	3
4	4	10	400	800	4
Total		170	–	–	–

C_{FW} = 0 ppm, $C_{R,out}$ = 5 ppm, $C_{T,out}$ = 10 ppm, C_D^{max} = 20 ppm.

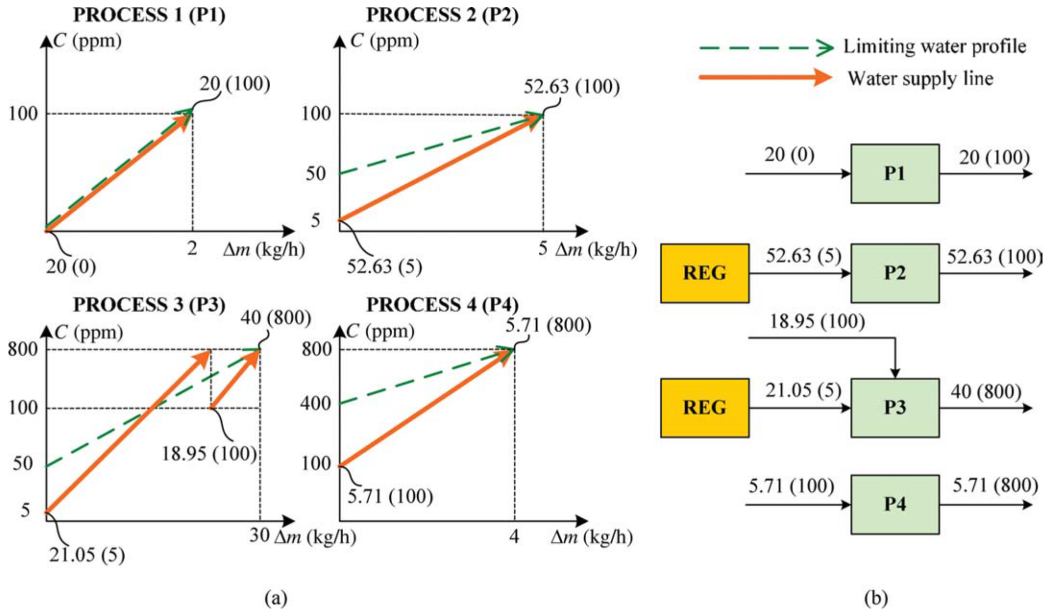

Figure 18. (a) Targeting for water system with regeneration reuse/recycle; (b) Water network design for Example 2.

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

(250 ppm) before it is being mixed with the bypass wastewater stream (0.15 t/h, 1000 ppm) for final discharge. The discharge concentration achieves the maximum discharge concentration at 300 ppm. The results for the various scenarios in this example are summarized in Table 2.

Example 2—Fixed load problem

A literature example taken from Wang and Smith[3] is solved to illustrate the application of PGA for the synthesis of total water network for FC problem. Table 3 shows the limiting data for four water-using processes with single contaminant constraint. In this example, pure freshwater is available for use. In this example, a fixed outlet concentration regeneration unit of 5 ppm used to regenerate water sources for further recovery.[3,21,27]

Following the proposed PGA approach, the allocations of all water sources for each process are first constructed and are shown in Figure 18. As shown, P1 is fed with freshwater and due to its limiting inlet concentration of 0 ppm. P2 is fed with regenerated water since its concentration (5 ppm) is lower than the limiting inlet concentration of P2 (50 ppm). Both processes then generated 72.63 t/h of internal water source of 100 ppm, which are reused in P3 (18.95 t/h) and P4 (5.71 t/h). Note that in P3, 21.05 t/h of regenerated water is also used to supplement the internal water source. The minimum freshwater and regeneration flow rates are targeted as 20 t/h and 73.68 t/h, respectively. Next, the revised

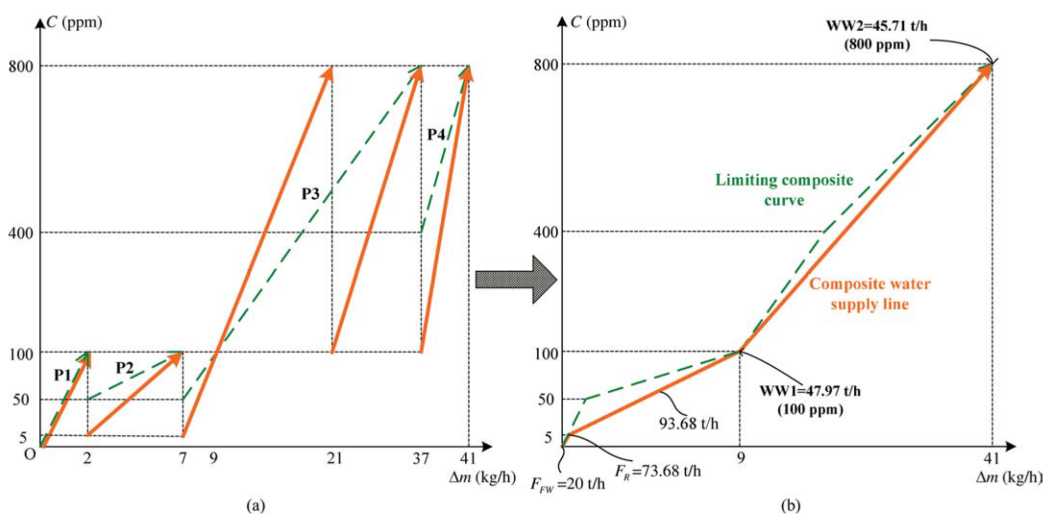

Figure 19. (a) Individual limiting water profiles and water supply lines for all water-using processes; (b) Limiting composite curve and composite water supply line for Example 2.

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

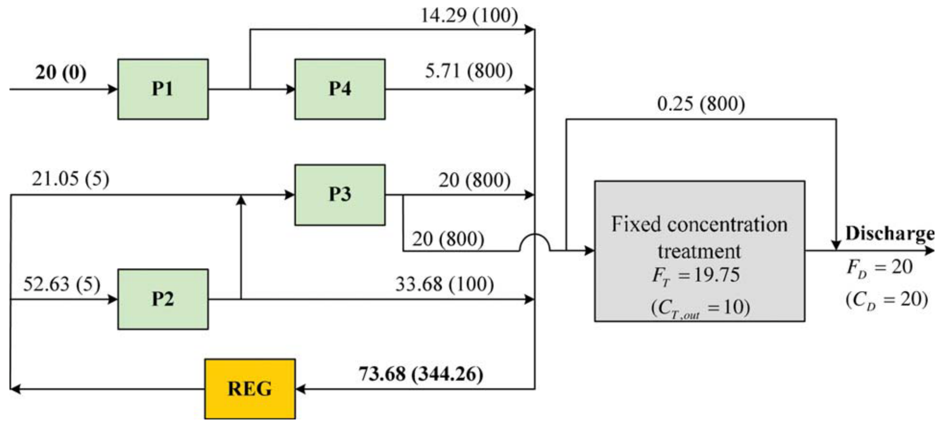

Figure 20. Total water network for Example 2.

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

limiting composite curve is constructed as shown in Figure 19. Note that there are two turning points at 5 ppm and 100 ppm in the composite water supply line where the pinch concentrations are located. Note also that pinch point at 5 ppm corresponds to the use of the regenerated water. Since 73.68 t/h of regenerated water is added into the water system at 5 ppm, the slope of the composite water supply line decreases sharply at this point. On the other hand, two wastewater streams are targeted, with flow rates of 47.97 t/h (WW1, 100 ppm) and 45.71 t/h (WW2, 800 ppm) respectively, indicated by the slope changes at the 100 ppm pinch concentration as well as the terminal point of the limiting composite curve. In order to minimize the regeneration mass load, wastewater of lower concentration, i.e. WW1 (47.97 t/h, 100 ppm) is first selected for regeneration. However, as the flow rate of WW1 is less than the targeted regeneration flow rate, additional 25.71 t/h (= 73.68 t/h − 47.97 t/h) of WW2 (800 ppm) is required for regeneration. This corresponds to the inlet concentration of regeneration as 344.26 ppm (C_{in}). Hence, Eq. 10 determines the minimum regeneration mass load (Δm_{R}) as 24.997 kg/h. On the other hand, the residual 20 t/h of WW2 (800 ppm) is sent for waste treatment before final discharge. It is worth mentioning that the water flow rate targets are identical with those reported in the literatures.[21,27]

To synthesize a total water network, a waste treatment system with $C_{\text{T,out}}$ of 10 ppm is taken into consideration. The maximum allowable discharge concentration ($C_{\text{D}}^{\max}$) in this example is given as 20 ppm. Solving Eq. 15 determines that the maximum discharge mass load (m_{D}) as 0.4 kg/h. Since pure fresh water is used, Δm_{FW} is set to zero. Based on Eqs. 10 and 14, Δm_{R} and Δm_{p} values are calculated as 24.997 kg/h and 41 kg/h, respectively. Consequently, the minimum treatment mass load (Δm_{T}) is determined as 15.603 kg/h from Eq. 12. As mentioned previously, the discharge flow rate (F_{D}) is originated from WW2, with flow rate of 20 t/h (800 ppm). Hence, this single waste stream is sent for final treatment, with the inlet treatment concentration identified as 800 ppm ($C_{\text{T,in}}$). Next, by solving Eq. 11, the minimum treatment flow rate is determined as 19.75 t/h. Figure 20 shows the total water network design for Example 2.

For comparison purpose, the water flow rate targets for direct reuse/recycle and regeneration schemes of this example[42] are also summarized in Table 4. Note that the targeted freshwater and regeneration flow rates for all schemes are

Table 4. Summary of the Targeting Results for Different Schemes (Example 2)

Schemes	Freshwater Flow Rate F_{FW} (t/h)	Regenerated Water Flow Rate F_{R} (t/h)	Minimum Treatment Flow Rate F_{T} (t/h)	Waste Stream	Contaminant Mass Load (kg/h): Freshwater m_{FW}	Water-Using Processes Δm_{p}	Regeneration Unit Δm_{R}	Treatment Unit Δm_{T}	Wastewater Discharge m_{D}
Reuse/recycle	90	–	–	WW1 (44.29 t/h, 100 ppm) WW2 (45.71 t/h, 800 ppm)	0	41	–	–	41
Reuse/recycle scheme by Ng et al.[27]	90	–	80	WW1 (44.29 t/h, 100 ppm) WW2 (45.71 t/h, 800 ppm)	0	39.2	–	39.2	–
Regeneration Reuse/recycle	20	73.68	–	WW (20 t/h, 800 ppm)	0	41	24.997	–	16
Total water network	20	73.68	19.75	WW (20 t/h, 20 ppm)	0	41	24.997	15.603	0.4
Total water network by Ng et al.[27]	20	73.68	17.79	WW1 (3.69 t/h, 100 ppm) WW2 (16.32 t/h, 800 ppm)	–	40.59	27.57	13.02	0.4

Table 5. Limiting Data for Example 3[7]

Process	Δm_i (kg/h)	$F^{\lim}_{i,\mathrm{in}}$ (t/h)	$F^{\lim}_{i,\mathrm{out}}$ (t/h)	$C^{\max}_{i,\mathrm{in}}$ (ppm)	$C^{\max}_{i,\mathrm{out}}$ (ppm)	Process Sequence i
1	1.5	50	50	20	50	1
2	5.0	100	100	50	100	2
3	4.0	80	70	100	150	3
4	3.5	70	60	200	250	4
Total		300	280	–	–	

$C_{FW(1)} = 0$ ppm, $C_{FW(2)} = 20$ ppm, $C_{FW(3)} = 50$ ppm, $C_{T,out} = 25$ ppm, $C^{\max}_{\mathrm{D}} = 30$ ppm.

identical to the previous reported studies.[21,27] However, the minimum treatment flow rate and the mass load removal in regeneration and treatment units are slightly different from the previous study.[27] As shown in Table 4, the results reported by Ng et al.[27] and PGA are shown in the last two rows. It is noted that the targeted flow rates for freshwater and regenerated water are the same. Besides, the mass load balance for all the water-using processes are almost the same and the

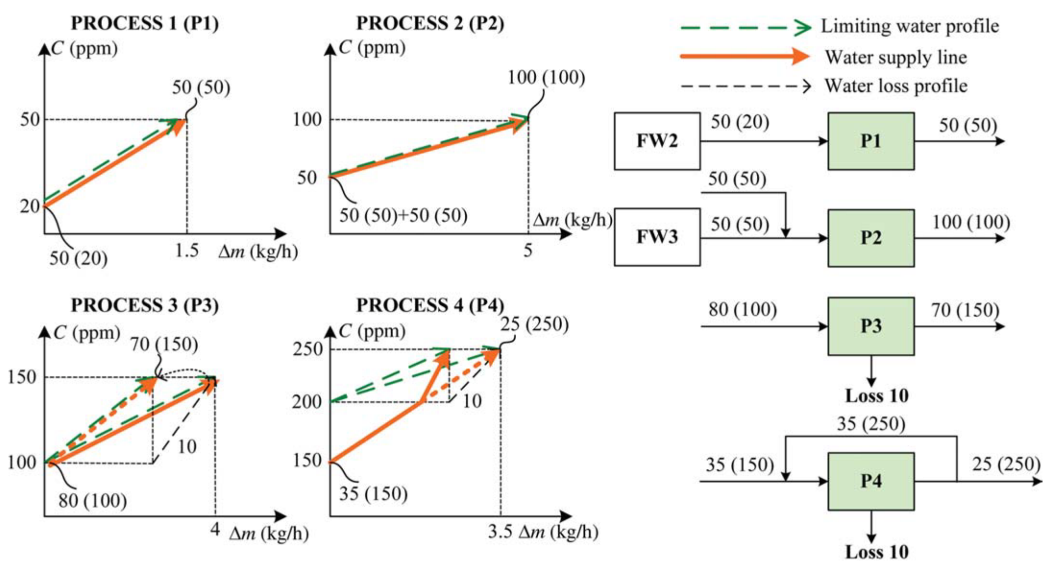

Figure 21. (a) Targeting for water system involving multiple water resources; (b) Water reuse/recycling network design for Example 3.

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

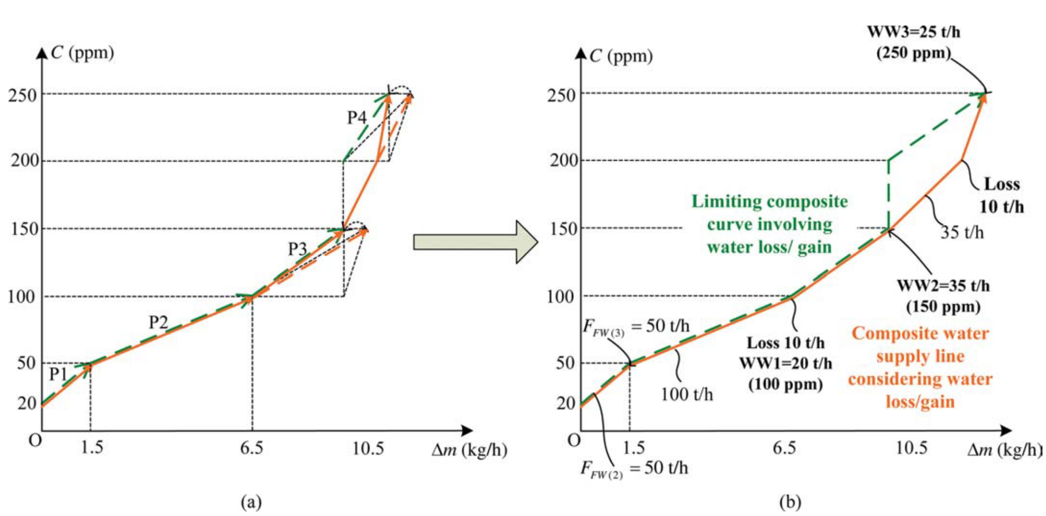

Figure 22. (a) Optimal water supply lines for water-using processes; (b) Composite water supply line for Example 3.

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

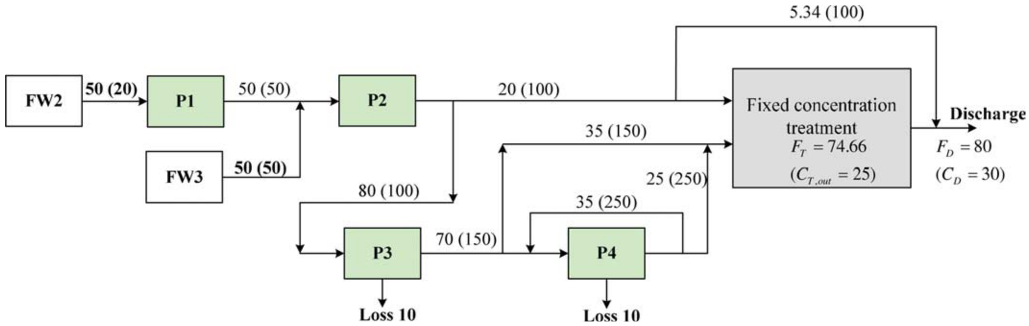

Figure 23. Optimal water network for Example 3.

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

tolerance is acceptable. It is interesting to note that the regeneration mass load targeted by PGA (24.997 kg/h) is smaller than the literature result (27.57 kg/h).[27] Meanwhile, the treatment mass load of PGA (15.603 kg/h) is higher than the literature (13.02 kg/h)[27] which leads to higher treatment flow rate. Although there are some variations in the individual regeneration and treatment load between both studies, the total mass load removal in the regeneration and treatment units in both solutions remain the same. This means that the problem is degenerate where multiple solutions are possible. Selection of optimum scheme is dependent on detailed cost analysis, which is beyond the scope of this work.

Example 3—Multiple external water resources

Table 5 shows the limiting data taken from Polley and Polley.[7] This example is used to illustrate the capability of proposed PGA in synthesizing a water network with water loss and multiple external water sources. The latter are having concentrations of 0 ppm (FW1), 20 ppm (FW2), and 50 ppm (FW3),[14] respectively. The main assumption for this example is that, the unit costs for sources of higher quality are much higher than those of lower quality (e.g., unit cost for FW1 is several magnitude more than that of FW2, etc.). For water sources of similar unit costs, the prioritized cost concept[16] should be embedded in the analysis. In this example, no regeneration system is taken into consideration. Meanwhile, the maximum allowable discharge concentration and waste treatment outlet concentration are given as 30 ppm (C_D^{max}) and 25 ppm ($C_{T,out}$), respectively.

Following the proposed PGA approach, water allocation for all water-using processes is shown in Figure 21. As shown, P1 and P2 are fed by FW2 and FW3 respectively, as their concentrations match the limiting inlet concentrations of P1 and P2. Effluent from these processes becomes the internal water sources of 50 and 100 ppm respectively. The latter is then reused in P3 (80 t/h), which then generates another internal water source of 150 ppm (70 t/h). A portion of this internal water source (35 t/h) is then reused in P4. The result indicates that the use of FW1 is not required as 50 t/h of FW2 and FW3 respectively are sufficient to fulfill the requirement of the water-using processes. The targeted results are the same with those reported in the literature.[14] The limiting composite curve and composite water supply line of Example 3 are shown in Figure 22.

In addition, three waste streams, WW1 (20 t/h, 100 ppm), WW2 (35 t/h, 150 ppm), and WW3 (25 t/h, 250 ppm) are identified based on the proposed PGA. Without considering the regeneration system, 20 t/h of WW1, 35 t/h of WW2 and 25 t/h of WW3 are sent for treatment for final discharge. Note that contaminant concentrations of WW1, WW2, and WW3 are higher than discharge limitation; therefore, all the waste streams require treatment before being discharged to the environment. Note that the total flow rate of wastewater for discharge (F_D) is determined via Eq. 16 as 80 t/h. With the discharge limit of 30 ppm, the wastewater streams have a total impurity load (m_D) of 2.4 kg/h (calculated using Eq. 15). As regeneration process is not considered in this example, Δm_R value is taken as zero. Next, m_{FW} and Δm_p values are calculated via Eqs. 13 and 14 as 3.5 kg/h and 10 kg/h,

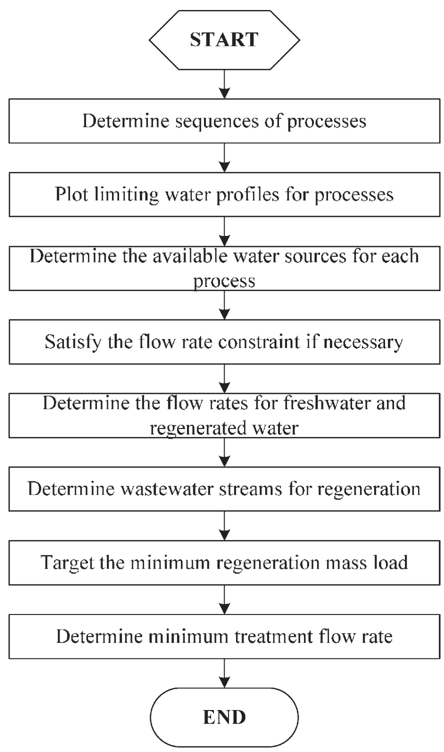

Figure 24. The heuristic design procedure for total water network.

respectively. Consequently, the minimum treatment mass load (Δm_T) is determined as 11.1 kg/h using Eq. 12. Meanwhile, following the wastewater targeting approach proposed of Ng et al.,[28] the minimum wastewater treatment flow rate is determined as 74.66 t/h, which means 5.34 t/h wastewater is bypassing the treatment unit. Figure 23 shows the water network design for Example 3, as the results of PGA.

Summary

All the proposed procedures presented earlier are generalized in a flow chart in Figure 24. Based on the given limiting data, the sequence of processes is first determined. Next, the limiting water profiles are plotted for processes. For each process, the appropriate water sources are determined. In case a FF process is involved, the FF constraint is satisfied. Next the flow rate targets for freshwater and regenerated water are located. Besides, the wastewater streams are also identified. By selecting the appropriate wastewater streams for regeneration, the regeneration mass load can be minimized. The unutilized wastewater (for regeneration) is then sent for wastewater treatment for final discharge. The minimum treatment and bypass flow rates can then be determined. Following the proposed approach, a total water network can be synthesized.

Conclusions

A newly proposed procedure called the PGA for simultaneous targeting and design of water network is proposed in this work. In this study, the revised limiting water profiles for water-using processes involving water loss/gain are proposed to locate the minimum water flow rates. The proposed PGA is applicable for both fixed load (with water loss/gain and FF constraints) and FF problems, and it can be used to synthesize water network that involves direct reuse/recycle, regeneration, and waste treatment (total water network), with single and multiple freshwater sources.

Acknowledgments

Financial support provided by the National Natural Science Foundation of China under Grant No. 20936004 is gratefully acknowledged. Sponsorship from the Malaysian Ministry of Science, Technology and Innovation via Science Fund (No. 0302-12-SF0018) is deeply appreciated.

Notation

$C_{i,\text{in}}^{\max}$ = limiting inlet concentration of process i
$C_{i,\text{out}}^{\max}$ = limiting outlet concentration of process i
$C_{i,\text{in}}^{\text{mix}}$ = mixed inlet concentration of process i
$C_{\text{FW}(k)}$ = concentration of the kth freshwater resource
$C_{\text{R,in}}$ = inlet concentration of regeneration process
$C_{\text{R,out}}$ = outlet concentration of regeneration process
$C_{\text{T,in}}$ = inlet concentration of treatment process
$C_{\text{T,out}}$ = outlet concentration of treatment process
C_{D} = contaminant mean concentration of discharge waste streams
$C_{\text{D}}^{\max}$ = the maximum allowable discharge concentration
$F_{i,\text{in}}^{\lim}$ = limiting inlet water flow rate of process i
$F_{i,\text{out}}^{\lim}$ = limiting outlet water flow rate of process i
$F_{i,\text{in}}$ = optimal water supply flow rate of process i
$F_{i,\text{out}}$ = the outlet water flow rate of process i
F_i^{loss} = water loss flow rate for process i
F_i^{gain} = water gain flow rate from process i
ΔF_{p} = overall flow rate difference for all the water-using processes
$F_{\text{FW},i}$ = flow rate of freshwater allocated to process i
$F_{\text{FW}(k)}$ = optimal flow rate for the kth water resource
F_{R} = optimal regeneration flow rate
F_{D} = flow rate of discharge waste streams
F_{T} = minimum treatment flow rate
$F_{WW(w)}^{\text{D}}$ = flow rate for the wth wastewater stream for treatment/discharge
FW = freshwater resource
i = index of the water-using processes
k = index of the external water sources
m_{FW} = total mass load for all water resources
m_{D} = mass load for discharge waste streams
Δm_i = given or pseudo-mass load difference for water-using process i
Δm_i^{net} = the net mass load difference for water-using process i
Δm_i^{gain} = the mass load difference for water-using process i with or without considering water gain
Δm_i^{loss} = the mass load difference for water-using process i with or without considering water loss
Δm_{R} = mass load for regeneration process
Δm_{T} = mass load for treatment process
Δm_{p} = overall mass load difference across all the water-using operations
N_{P} = total number for the water-using processes
N_{S} = total number for external water sources or resources
N_{R} = total number for in-plant regeneration processes
N_{T} = total number for end-of-pipe treatment processes
PGA = process-based graphical approach
REG = regeneration process
RR = removal ratio
r = index of the regeneration processes
t = index of the treatment processes
WPD = water profile diagram
WW = wastewater stream

Literature Cited

1. Hallale N. A new graphical targeting method for water minimisation. *Adv Environ Res.* 2002;6:377–390.
2. Manan ZA, Tan YL, Foo DCY. Targeting the minimum water flow rate using water cascade analysis technique. *AlChE J.* 2004;50:3169–3183.
3. Wang YP, Smith R. Wastewater minimisation. *Chem Eng Sci.* 1994;49:981–1006.
4. Wang YP, Smith R. Wastewater minimization with flowrate constraints. *Chem Eng Res Des.* 1995;73:885–900.
5. Mann JG, Liu YA. *Industrial Water Reuse and Wastewater Minimization*. New York: McGraw-Hill, 1999.
6. Dhole VR, Ramchandani N, Tainsh RA, Wasilewski M. Make your process water pay for itself. *Chem. Eng.* 1996;103:100.
7. Polley GT, Polley HL. Design better water networks. *Chem Eng Prog.* 2000;96:47–52.
8. El-Halwagi MM, Gabriel F, Harell D. Rigorous graphical targeting for resource conservation via material recycle/reuse networks. *Ind Eng Chem Res.* 2003;42:4319–4328.
9. Almutlaq AM, Kazantzi V, El-Halwagi MM. An algebraic approach to targeting waste discharge and impure fresh usage via material recycle/reuse networks. *Clean Technol Environ Policy.* 2005;7:294–305.
10. Prakash R, Shenoy UV. Targeting and design of water networks for fixed flowrate and fixed contaminant load operations. *Chem Eng Sci.* 2005;60:255–268.
11. Foo DCY, Manan ZA, Tan YL. Use cascade analysis to optimize water networks. *Chem Eng Prog.* 2006;102:45–52.
12. Alwi SRW, Manan ZA. Generic graphical technique for simultaneous targeting and design of water networks. *Ind Eng Chem Res.* 2008;47:2762–2777.
13. Foo DCY. Flowrate targeting for threshold problems and plant-wide integration for water network synthesis. *J Environ Manage.* 2008;88:253–274.
14. Foo DCY. Water cascade analysis for single and multiple impure fresh water feed. *Chem Eng Res Des.* 2007;85:1169–1177.

15. Alwi SRW, Manan ZA. Targeting multiple water utilities using composite curves. *Ind Eng Chem Res.* 2007;46:5968–5976.
16. Shenoy UV, Bandyopadhyay S. Targeting for multiple resources. *Ind Eng Chem Res.* 2007;46:3698–3708.
17. Kuo WCJ, Smith R. Design of water-using systems involving regeneration. *Process Saf Environ.* 1998;76:94–114.
18. Feng X, Bai J, Zheng XS. On the use of graphical method to determine the targets of single-contaminant regeneration recycling water systems. *Chem Eng Sci.* 2007;62:2127–2138.
19. Bai J, Feng X, Deng C. Graphically based optimization of single-contaminant regeneration reuse water systems. *Chem Eng Res Des.* 2007;85:1178–1187.
20. Agrawal V, Shenoy UV. Unified conceptual approach to targeting and design of water and hydrogen networks. *AlChE J.* 2006;52: 1071–1082.
21. Ng DKS, Foo DCY, Tan RR, Tan YL. Ultimate flowrate targeting with regeneration placement. *Chem Eng Res Des.* 2007;85:1253–1267.
22. Wang YP, Smith R. Design of distributed effluent treatment systems. *Chem Eng Sci.* 1994;49:3127–3145.
23. Kuo WCJ, Smith R. Effluent treatment system design. *Chem Eng Sci.* 1997;52:4273–4290.
24. Kuo WCJ, Smith R. Designing for the interactions between water-use and effluent treatment. *Chem Eng Res Des.* 1998;76:287–301.
25. Bandyopadhyay S, Ghanekar MD, Pillai HK. Process water management. *Ind Eng Chem Res.* 2006;45:5287–5297.
26. Ng DKS, Foo DCY, Tan RR. Targeting for total water network. 1. Waste stream identification. *Ind Eng Chem Res.* 2007;46:9107–9113.
27. Ng DKS, Foo DCY, Tan RR. Targeting for total water network. 2. Waste treatment targeting and interactions with water system elements. *Ind Eng Chem Res.* 2007;46:9114–9125.
28. Linnhoff B, Townsend D, Boland D, Hewitt G, Thomas B, Guy A, Marsland R. *User Guide on Process Integration for the Efficient Use of Energy*, *1st ed.* Rugby, U. K.: IChemE, 1982.
29. Smith R. *Chemical Process Design and Integration*, *2nd ed.* Wiley, 2005.
30. Kemp I. *Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy*, *2nd ed.* Oxford, U. K.: Butterworth-Heinemann Ltd, 2007.
31. El-Halwagi MM. *Process Integration.* San Diego: Academic Press, 2006.
32. Feng X, Seider WD. New structure and design methodology for water networks. *Ind Eng Chem Res.* 2001;40:6140–6146.
33. Gomes JFS, Queiroz EM, Pessoa FLP. Design procedure for water/wastewater minimization: single contaminant. *J Cleaner Prod.* 2007; 15:474–485.
34. El-Halwagi MM. *Pollution Prevention through Process Integration: Systematic Design Tools.* San Diego: Academic Press, 1997.
35. Foo DCY. Letter to the editor. *AlChE J.* 2010;56:2492–2494.
36. Prakash R, Shenoy UV. Design and evolution of water networks by source shifts. *Chem Eng Sci.* 2005;60:2089–2093.
37. Ng DKS, Foo DCY. Evolution of water network using improved source shift algorithm and water path analysis. *Ind Eng Chem Res.* 2006;45:8095–8104.
38. Das AK, Shenoy UV, Bandyopadhyay S. Evolution of resource allocation networks. *Ind Eng Chem Res.* 2009;48:7152–7167.
39. Foo DCY. State-of-the-art review of pinch analysis techniques for water network synthesis. *Ind Eng Chem Res.* 2009;48:5125–5159.
40. Jeżowski J, Poplewski G, Jeżowska A. Optimization of water usage in chemical industry. *Environ Protect Eng.* 2003;29:97–117.
41. Deng C, Feng X, Bai J. Graphically based analysis for water system with zero liquid discharge. *Chem Eng Res Des.* 2008;86:165–171.
42. Deng C, Feng X, Ng DKS, Foo DCY. Process-based graphical approach (PGA) for simultaneous targeting and design of regeneration recycling water networks. *Proceedings of the 12th Asia Pacific Confederation of Chemical Engineers (APCChE 2008)*, Dalian, China, 2008.

Manuscript received May 2, 2009, and and revision received Nov. 11, 2010.