Optimal Design of Single-Contaminant Regeneration Reuse Water Networks with Process Decomposition

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Water network with regeneration schemes (e.g., regeneration reuse, regeneration recycling) can reduce freshwater consumption further than water network merely with direct reuse. Regeneration reuse, compared with regeneration recycling, can additionally avoid unexpected accumulation of contaminants. Owing to these features, process decomposition can help to reduce freshwater usage and wastewater discharge of regeneration reuse water systems and achieve the results, which graphical method delivers. In this article, the effect of decomposition on water-using process and further on regeneration reuse water system is briefly analyzed on the concentration-mass load diagram. Then a superstructure and three sequential mathematical models, which take process decomposition into account, are in turn developed to optimize single contaminant regeneration reuse water systems. By several examples, the reliability of the models is verified. Moreover, several decomposition strategies are summarized to realize the regeneration reuse water network, which attains the targets from graphical method. The results indicate that postregeneration concentration has a major impact on the scheme of process decomposition.
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Introduction

Recently, with increasing stringent emission control regulations and serious water scarcity around the world, much more attention has been paid to minimize wastewater generation and freshwater consumption from both industry and academic community. Bagajewicz[1] reviewed the milestone and main works on design and retrofit of water networks in 2000. Over the past decades, numerous works have been conducted to synthesis water network via conceptual approaches[2–16] or mathematical modeling.[17–30]

After the water recovery possibility has been exhausted via water direct reuse,[2,5–7] regeneration is turned to further reduce the freshwater intake and wastewater discharge of a water system. Regeneration recycling and regeneration reuse, as two essential schemes involving regeneration unit, are quite attractive on water minimization. For regeneration recycling, wastewater is totally treated and recycled, thus it can achieve maximum water reutilization.[2,5,10,12-16,25,29] However, the regenerated water can re-enter the processes in which it has been previously used, unexpected accumulation of contaminants exists and shadows the advantage of regeneration recycling. As a tradeoff, regeneration reuse takes advantage of the treatment process, and simultaneously avoids the recycle of regenerated water, thus more study on regeneration reuse has been carried out in recent years.[2-5,11,24,26]

Research on regeneration reuse water networks generally resorts to two traditional approaches: graphical method and mathematical programming. Nearly all the attempts with graphical method[3-5,11] are based on the water pinch technology

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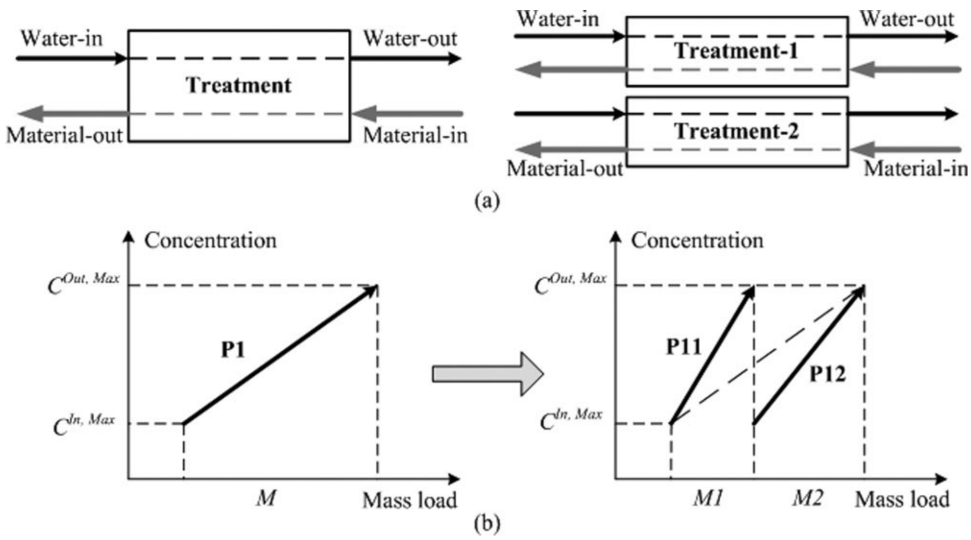

Figure 1. (a) Mass load decomposition of practical water-using process; (b) graphical representation for mass load decomposition.

introduced by Wang and Smith.[2] The graphical method as a conceptual approach can be used to target the freshwater usage of a single-contaminant water system, but the resultant network cannot be obtained automatically. As a result, most research on optimization and design of regeneration reuse water networks leans towards the use of mathematical programming.

As for mathematical programming, regeneration reuse, as one of the possibilities to reduce the freshwater consumption or total cost of a water system, is generally incorporated into a certain superstructure. The targeting and design of regeneration reuse options can be simultaneously carried out by solving the corresponding mathematical models.[17,18,22,27,31] Besides, several researchers also put forward the optimizing models exclusively for regeneration reuse. Bagajewicz and Savelski[20] presented a MILP model for optimizing single-contaminant regeneration reuse water systems at a certain postregeneration concentration by utilizing the necessary conditions of optimality. Xu et al.[24] studied the relationship between optimal regeneration concentration and pinch concentration on the basis of sequential optimization for single-contaminant systems. Later, they proposed a sequential-operation-model-based, global optimization method for the design of single-contaminant regeneration reuse water networks.[26] In the article, three cases considering the decomposition of water-using processes were discussed, and the corresponding design procedures were addressed targeting minimum freshwater and regenerated water usage.

To sum up, the research to date on regeneration reuse water systems is comparatively limited, and there are still problems that require further attention.

Firstly, process decomposition can further reduce the freshwater consumption of a regeneration reuse water system, which has been manifested in some available research.[4,20] However, why and how does process decomposition influence the targets and resultant network of a regeneration reuse water system still remains unaccounted.

Secondly, graphical method, which essentially supposes that each water-using process is decomposable, can deliver the targets of a single-contaminant regeneration reuse water system.[11] However, mathematical models in most available research actually consider each process as a whole.[18,20-22,24,26-30] As a result, the corresponding network often cannot attain the targets determined by the graphical method. Methodology and strategy for designing the regeneration reuse water network, which is in line with the targets from graphical method, are actually another pending problem.

All these problems will be considered in this article. The graphical method in our previous article [11] renders the primary targets of a single-contaminant regeneration reuse water system, including freshwater consumption, regenerated water flow rate and contaminant regeneration load.[11] This article aims at constructing the corresponding network by the aid of mathematical programming. The sequential optimization methodology adopted in graphical analysis will be extended to the construction of mathematical models.

Regeneration Reuse and Research Objective

Regeneration reuse

Regeneration reuse is categorized into total regeneration and partial regeneration. For total regeneration, all the water, when the concentrations reach the regeneration concentrations, is sent to regeneration unit for treatment. Thus the flow rate of regenerated water is equal to that of freshwater, if water loss is ignored. While for partial regeneration, only partial amount of contaminated water is regenerated, and the residual wastewater is directly reused or discharged, which means that the regenerated water flow rate is smaller than the freshwater quantity. If regenerating part of water can meet the demand of a system, partial regeneration is undoubtedly utilized to guarantee a lower regeneration cost. Therefore, when designing water-using networks with regeneration reuse, it is essential to distinguish total and partial regeneration.

The water requirement of a regeneration reuse network is closely related to postregeneration concentrations. The lower is the postregeneration concentration; the smaller is the flow rate of freshwater and regenerated water.[11] In other words,

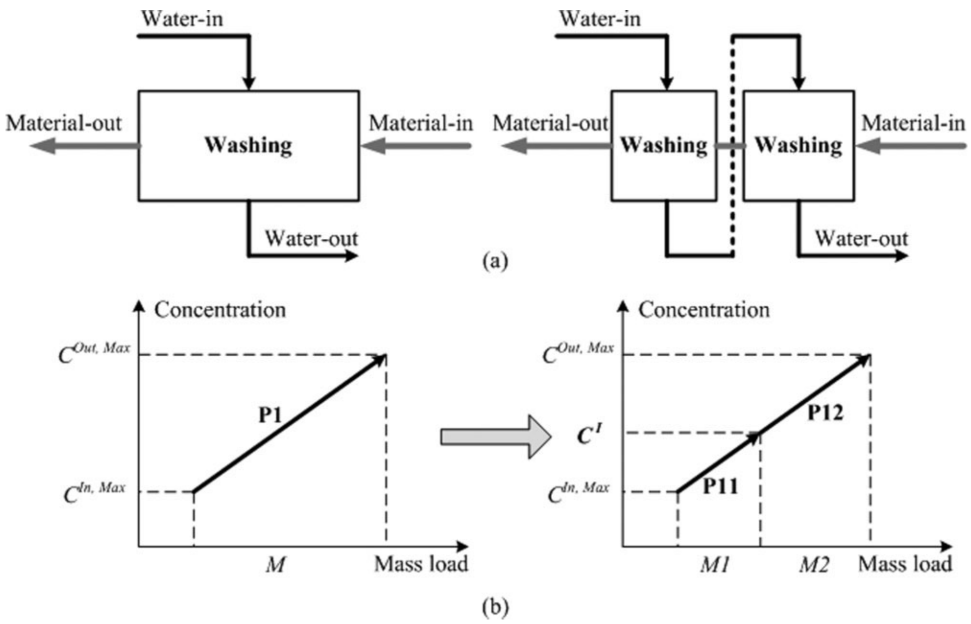

Figure 2. (a) Concentration decomposition of practical water-using process; (b) graphical representation for concentration decomposition.

the freshwater cost decreases, while the regeneration cost increases on account of stricter treatment requirements. Contrarily, a higher postregeneration concentration corresponds to a higher freshwater cost but a lower regeneration cost. Therefore, the determination of the optimal postregeneration concentration is actually an economic problem.[31] In this article, for the sake of exempting from complicated economic factors, the postregeneration concentration is taken to be a given parameter.

As we will discuss in the following sections, process decomposition affects the targets and configuration of a regeneration reuse water system. When designing a water-using network with regeneration reuse, process decomposition should be properly considered. Indeed, besides saving freshwater, the decomposition of processes will bring about a complex network structure and increasing capital cost. However, the freshwater reduction effect is mainly considered in this article to investigate how the decomposition schemes influence the network design results.

Research objective

This article mainly explores mathematical models for designing single-contaminant regeneration reuse water networks that allows design options with any types of process decomposition. Why and how process decomposition influences the targets of regeneration reuse water systems will be first discussed on the concentration-mass load diagram. Then mathematical models will be developed to incorporate process decomposition into network generation. Whether to implement total or partial regeneration, will be easily identified through optimization. And strategies for process decomposition will be summarized.

Table 1. Limiting Process Data For Example Case

Process	$C^{In,Max}$/ppm	$C^{Out,Max}$/ppm	Mass Load/kg h^{-1}
1	0	100	3.0
2	50	100	1.0
3	25	150	3.75

Process Decomposition

The regenerated water in regeneration reuse systems cannot be recycled. Thus for freshwater and wastewater minimization, some water-using processes are generally split in such a way that one subprocess is placed before the regeneration unit to remove part of contaminant load of the original process and the other is positioned after it to treat the

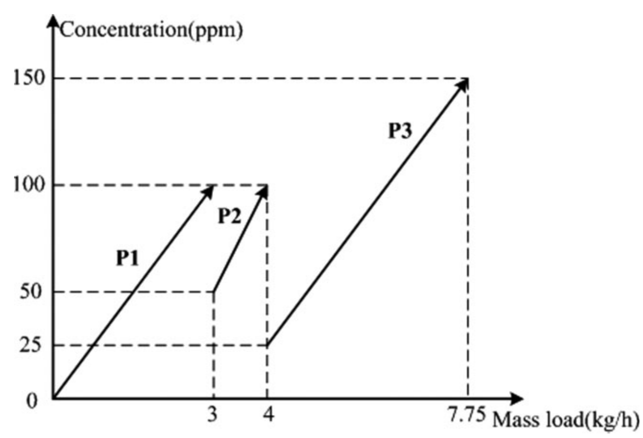

Figure 3. Limiting water profiles of the example system.

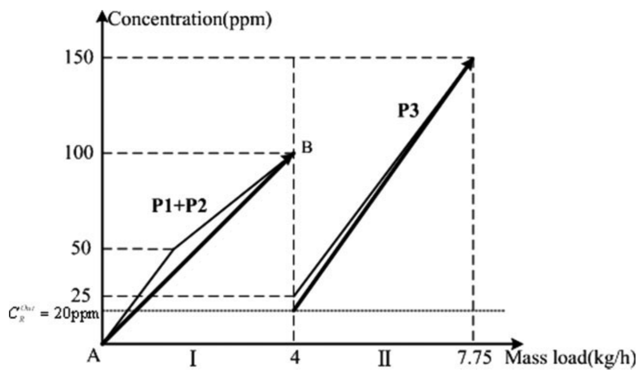

Figure 4. Target freshwater without process decomposition.

remaining load. In this way, more water saving possibilities will occur.

There are mainly two kinds of process decomposition, mass load decomposition (parallel connection), and concentration decomposition (series connection). Disposing wastewater in batches is actually mass load decomposition of wastewater treatment process, while multistage washing-up belongs to concentration decomposition. The two types of decomposition have different features, thus when imposed on water-using processes, the water usage and the configuration of water networks will be different. The effect of decomposition on water-using processes and further on regeneration reuse water systems can be analyzed on the concentration-mass load diagram. Considering the complexity, necessity, and feasibility of decomposition, a water-using process is at most split into two subprocesses in this article.

Mass load decomposition

By allocating contaminant mass load, a water-using process, such as extraction, absorption, and washing with water as mass transfer agent, can be decomposed into two subprocesses. As shown in Figure 1a, a water treatment process is split into two units, which in practice means the wastewater is treated in two batches. Such a case can be taken as an example for mass load decomposition. The corresponding graphical representation is illustrated in Figure 1b by the well-known concentration-mass load diagram proposed by Wang and Smith.[2] Note that the two subprocesses P11 and P12 are operated in parallel and independent from each other. As shown in Figure 1b, the limiting inlet and outlet concentrations of P11 and P12 are both identical to those of the original process. In addition, the sum of mass loads of the subprocesses is equal to the mass load of the original process. The proportion of the contaminant mass load for one of the subprocesses (e.g., P11) is defined as splitting factor, which is denoted as α_1. Then the relations of parameters before and after the mass load decomposition can be expressed by the following expressions.

$$\begin{cases} M_1 = M \times \alpha_1 & M_2 = M \times (1-\alpha_1) \\ C_{11}^{\mathrm{In,Max}} = C_1^{\mathrm{In,Max}} & C_{11}^{\mathrm{Out,Max}} = C_1^{\mathrm{Out,Max}} \\ C_{12}^{\mathrm{In,Max}} = C_1^{\mathrm{In,Max}} & C_{12}^{\mathrm{Out,Max}} = C_1^{\mathrm{Out,Max}} \end{cases} \tag{1}$$

As shown in Figure 1b, the slope of the limiting water profiles for P11 and P12 are higher than that for P1, which means that the limiting water flow rates for P11 and P12 are smaller than that for P1. Thus the water flow rate limitation is slacked by the mass load decomposition.

It is worthy to mention that Wang and Smith[32] split a single process into two parts and then employed the reuse approach to satisfy flow rate requirements. The part with the smallest flow rate is fed with water firstly and the effluent incurred will be reused by the other part with higher flow rate. In this way, the flow rate requirements can be met. In fact, this splitting and reuse methodology is similar with the mass load decomposition proposed here.

Concentration decomposition

Multistage washing process is a classical case for concentration decomposition. Figure 2a shows how a single stage washing process is split into two stages in series and Figure 2b are the respective graphical representation before and after splitting. It can be seen that, water-using process P1 is split into two independent subprocesses (P11 and P12) with different limiting concentrations. The sum of mass loads of P11 and P12 is equal to the mass load of P1. Obviously, the limiting inlet concentration of P11 and the limiting outlet concentration of P12 are equal to the corresponding concentration of P1. The limiting outlet concentration of P11 is same as the limiting inlet concentration of P12. This special concentration is defined as interim concentration where the concentration decomposition for the process locates and denoted as C^I. It is worthy to mention that the splitting

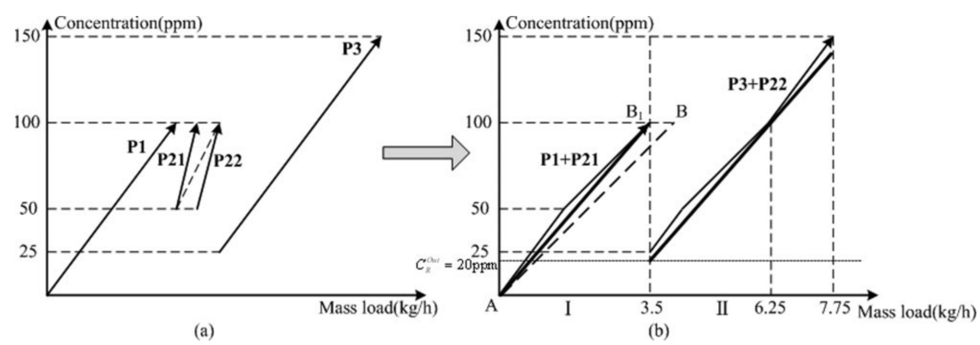

Figure 5. (a) Limiting water profiles considering mass load decomposition; (b) target freshwater with mass load decomposition of P2.

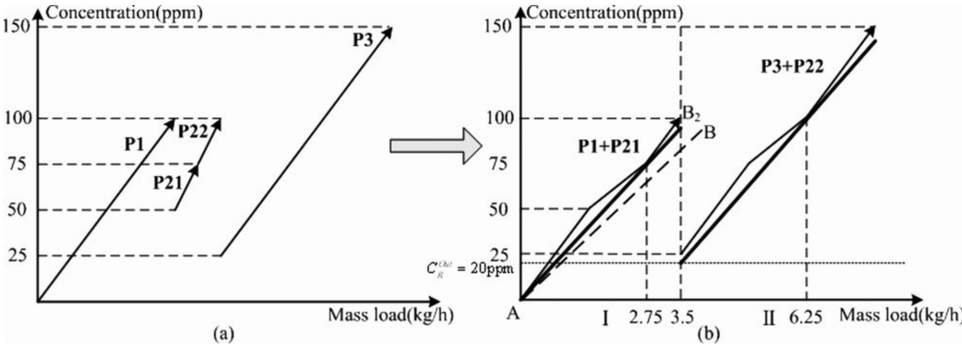

Figure 6. (a) Limiting water profiles considering concentration decomposition; (b) target freshwater with concentration decomposition of P2.

factor α_1 for concentration decomposition can be calculated with the interim concentration and limiting inlet and outlet concentrations of P1. The relations of parameters are described in the following expressions.

$$\begin{cases} M_1 = M \times \alpha_1 & M_2 = M \times (1 - \alpha_1) \\ C_{11}^{\text{In,Max}} = C_1^{\text{In,Max}} & C_{11}^{\text{Out,Max}} = C^I \\ C_{12}^{\text{In,Max}} = C^I & C_{12}^{\text{Out,Max}} = C_1^{\text{Out,Max}} \\ \alpha = (C^I C_{11}^{\text{In,Max}})/(C_1^{\text{Out,Max}} - C_1^{\text{In,Max}}) & \end{cases} \quad (2)$$

Noticeably, the limiting outlet concentration of P11 is less than that of P1, which means that more processes would reuse the outlet water from P11 other than P1. In addition, the limiting inlet concentration of P12 is higher than that of P1, which means that more water can be reused by P12 other than P1. Therefore, concentration decomposition improves the possibility of water reuse.

Effect of process decomposition on regeneration reuse system

Decomposition slacks the water quantity and quality requirements of water-using processes, and will further influence water demand of the whole system. Here a water system with three water-using processes (Table 1) is taken as an example to illustrate the effect of process decomposition on regeneration reuse water systems. Figure 3 shows the limiting water profiles of the three processes.

According to the features of regeneration reuse, Kuo and Smith[3] presented a grouping method to determine the freshwater target of a regeneration reuse water system, which can handily avoid the recycle of regenerated water and the decomposition of water-using processes. All the processes of a water-using system are divided into two subgroups. One group (Group I) is fed by fresh water and the other (Group II) is supplied by regenerated water from Group I. Hence, the flow rate of regenerated water should be less than or equal to that of freshwater. Here we will adopt the grouping method to target the freshwater usage of regeneration reuse water systems in the case of process decomposition.

When considering decomposition, one or several water-using processes are split first. Then take each process after decomposition as a certain and independent one, and group them.

For the water system in Figure 3, assume that the postregeneration concentration (C_R^{Out}) is 20 ppm. Let's analyze the case of no process decomposition. Apparently, water-using process P1 with its limiting inlet concentration less than C_R^{Out} has to use freshwater. For P2 and P3, the limiting inlet concentrations of which are greater than C_R^{Out}, either freshwater or regenerated water can be used. To minimize the freshwater consumption and maximize the regenerated water usage, P2 is combined with P1 in Group I. Then the optimal freshwater supply line (line AB in Figure 4) is determined by counterclockwise rotating the freshwater supply line until it touches the limiting composite curve in Group I. The freshwater flow rate then can be calculated as 40 t/h [= (4 kg/h) × 1000/(100 ppm–0 ppm)], and the corresponding regenerated flow rate is obtained as 30 t/h [= (7.75 kg/h-4 kg/h) × 1000/(150 ppm–20 ppm)].

Noticeably, mass load of P2 can be partially shifted to Group II to further reduce the freshwater consumption. Now consider mass load decomposition of P2. Assume the splitting factor is 0.5. Then there will be four processes in the system (P1, P21, P22, and P3), as shown in Figure 5a. These processes can be allocated in such a way that P1 and P21 are in Group I, and P3 and P22 in Group II. Then the freshwater supply line corresponds to line AB_1 (Figure 5b). Apparently the slope of line AB_1 is greater than that of line AB, thus the freshwater usage of the system decreases. Actually, the freshwater flow rate here is 35 t/h [= 3.5 kg/h × 1000/(100 ppm–0 ppm)] and the corresponding regenerated flow rate is 34.375 t/h [= (6.25 kg/h–3.5 kg/h) × 1000/

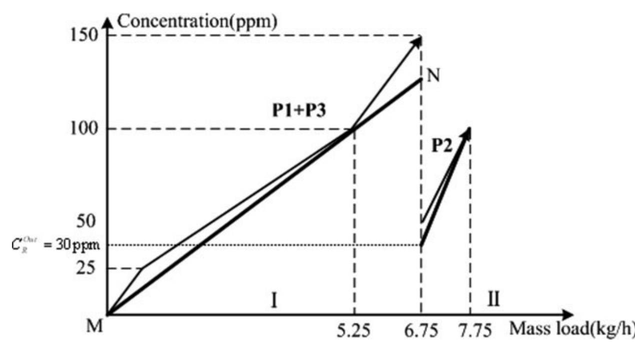

Figure 7. Target freshwater at a higher postregeneration concentration without process decomposition.

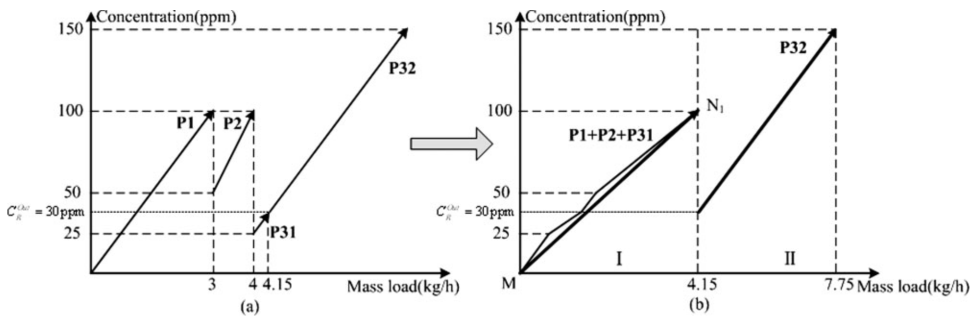

Figure 8. (a) Limiting water profiles considering concentration decomposition; (b) target freshwater at a higher postregeneration concentration with concentration decomposition of P3.

(100 ppm–20 ppm)]. Compared with the case without process decomposition (40 t/h), the freshwater usage here is reduced by 5 t/h due to mass load decomposition.

Similarly, in the case of concentration decomposition, P2 can be split into P21 and P22 with 75 ppm as the interim concentration as shown in Figure 6a. The splitting factor for concentration decomposition can be calculated as 0.5 by solving Eq. 2. The subprocess P21 with lower concentration interval is placed in Group I, and P22 with higher concentration locates in Group II. As shown in Figure 6b, the freshwater usage is determined by the reciprocal of the slope of line AB_2. Since the slope of line AB_2 is greater than that of line AB, concentration decomposition also reduces the freshwater expenditure of the system. By calculation, the freshwater flow rate is 36.67 t/h [= 2.75 kg/h $\times$ 1000/(75 ppm-0)], and the corresponding regenerated flow rate is 34.375 t/h [= (6.25 kg/h–3.5 kg/h) $\times$ 1000/(100 ppm-20 ppm)]. Hence 3.33 t/h (= 40 t/h–36.67 t/h) freshwater is reduced by concentration decomposition. Noticeably, the freshwater decrement from concentration decomposition (3.33 t/h) is smaller than that from mass load decomposition (5 t/h).

In the earlier discussion, the postregeneration concentration is taken to be 20 ppm, which is lower than 25 ppm, the second lowest limiting inlet concentration of the system. If the postregeneration concentration is higher, the advantage of concentration decomposition will specially prevail. Given the postregeneration concentration is 30 ppm. In this case, without considering process decomposition, P1 and P3 will be placed in Group I because their limiting inlet concentrations (0 ppm and 25 ppm) are lower than the postregeneration concentration (30 ppm), while P2 is located in Group II. Then the optimal freshwater supply line is determined by the limiting composite curve in Group I, as line MN shown in Figure 7, and the target freshwater flow rate is calculated as 52.5 t/h [= 5.25 kg/h $\times$ 1000/(100 ppm–0 ppm)]. Note that the postregeneration concentration (30 ppm) rightly falls into the limiting concentration interval (25 ppm, 150 ppm) of P3 and the limiting inlet concentration (25 ppm) of P3 is the second lowest inlet concentration of the water system. P3 is then applied for concentration decomposition with the postregeneration concentration as the interim concentration to reduce the freshwater intake. Actually, concentration decomposition by taking postregeneration concentration as the interim concentration has been considered by Xu et al.,[26] before. Here the validity and feasibility of this method will be further illustrated on the concentration-mass load diagram. P3 is split into two subprocesses P31 and P32 with the postregeneration concentration as the interim concentration. P1 and P31 are definitely placed in Group I while P32 is in Group II. Moreover, P2 is shifted from Group II to Group I to make sure the regenerated water flow rate does not exceed the freshwater flow rate. In this way, the freshwater consumption, which corresponds to the reciprocal of the slope of line MN_1 in Figure 8, can be calculated as 41.5 t/h [= 4.15 kg/h $\times$ 1000/(100 ppm–0 ppm)]. It is greatly decreased in comparison with freshwater consumption (52.5 t/h) in the case of no decomposition. What should be emphasized is that, this reduction cannot be achieved by mass load decomposition. That is because the P31 and P32 are separately located in Group I and Group II in the case of

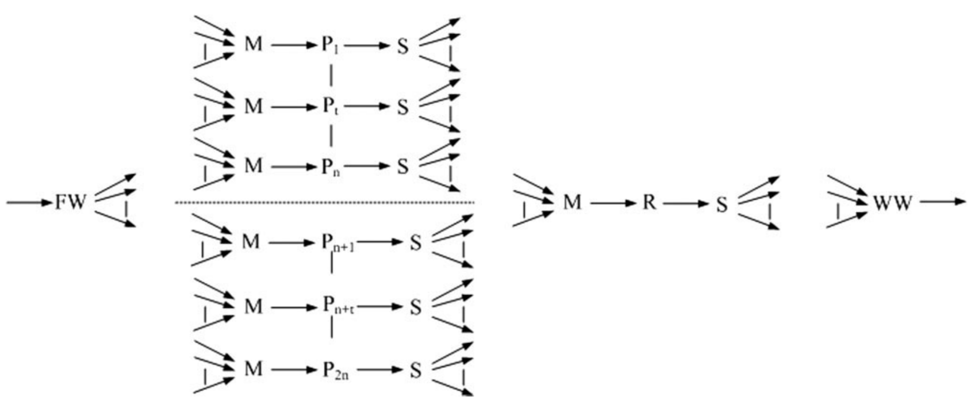

Figure 9. Superstructure of a typical regeneration reuse water network.

concentration decomposition that enables the contaminant mass load of the original process be removed by both freshwater and regenerated water. However, mass load decomposition fails to save the freshwater intake, because both of the subprocesses (P31 and P32) will still be in Group I, or in other words, fed by freshwater after decomposition.

On the whole, for a water-using system with regeneration reuse, process decomposition is an effective way for water minimization, no matter mass load or concentration decomposition is adopted. If the postregeneration concentration is higher than the second lowest limiting inlet concentration of the system (e.g., 25 ppm in the example water system), and the postregeneration concentration locates in the concentration interval of certain processes, it will be a wise choice to utilize the concentration decomposition on those processes for freshwater reduction. It is worthy to mention that, graphical analysis here only gives a rough insight into the effect of process decomposition on regeneration reuse systems. The detailed decomposition strategies for synthesizing the target regeneration reuse water network will be concluded by referring to mathematical programming.

Superstructure

Regeneration reuse is considered in water-using systems. Given are a set of water-using processes P ($P = \{t \in P | 1 \leq t \leq n\}$) which require water with a certain quality, and one regeneration unit which treats wastewater to a certain degree. For each water-using process, its inlet can be freshwater, used water from other processes or regenerated water, while at the outlet, the discharged water may be directly discharged to the end of pipe treatment, reused in other processes, or sent to the regeneration unit to treat. Note that, the water loss or gain in each process or the regeneration unit is ignored. In addition, a water-using process cannot receive water from and discharge water to the regeneration unit simultaneously. Since process decomposition should be considered when optimizing regeneration reuse water networks, here each water-using process (process t) is supposed to be split into two independent subprocesses (subprocesses t and $n+t$). As shown in Figure 9, process decomposition doubles the number of water-using processes in the system. The new set of water-using processes are defined as Q ($Q = \{1, \ldots t \ldots, n, n+1, \ldots n+t \ldots, 2n\}$) in the following discussion.

Figure 9 shows the superstructure of a water system with regeneration reuse, which embodies all possible configurations in design. The superstructure is developed as follows.

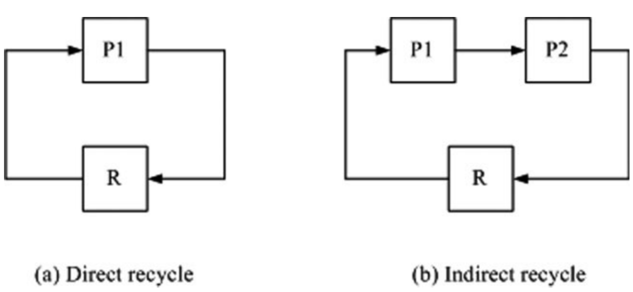

Figure 10. Forbidden configurations in regeneration reuse water networks.

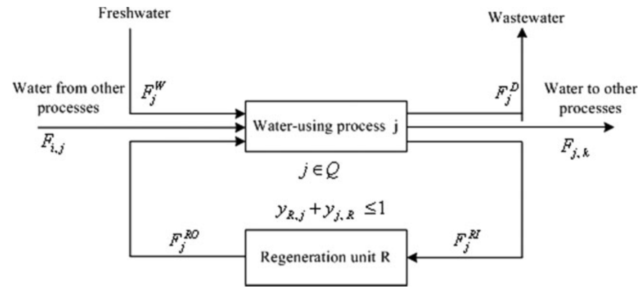

Figure 11. Nomenclature for water-using processes and regeneration unit.

(1) FW denotes the freshwater source. The arrows originating from it represent freshwater streams sent to water-using processes.

(2) P denotes water-using processes. Place a mixer node M before each water-using process. The water streams from the freshwater source, other processes and/or the regeneration unit are merged at the node and then sent to each process.

(3) R denotes the regeneration unit. Place a mixer node M before the regeneration unit. Arrows pointing to the mixer node represent streams from water-using processes.

(4) WW denotes the wastewater collector. The stream branches pointing to it represent the wastewater from water-using processes.

(5) Place a splitter node S after each water-using process P. Each process discharges its used water through the splitter, S, to the wastewater collector, other processes and/or the regeneration unit. In other words, the splitting branches of every such node can be connected to the mixer nodes established in step (2)–(4).

(6) Place a splitter node S after the regeneration unit R. Through the splitter S, water in the regeneration unit can be sent to any water-using processes, which means the connections between the splitting branches from such node and the mixer nodes in step (2).

(7) In view of the concept of regeneration reuse, if a process reuses the regenerated water from the regeneration unit, the discharged water from the process cannot re-enter the regeneration unit (direct recycle in Figure 10a), or reused in other processes, which take the regenerated water as a water source (indirect recycle in Figure 10). Note that only two processes involved indirect recycle is presented here for simplicity.

For a better understanding of the network superstructure, Figure 11 summarizes the nomenclature for water-using processes and the regeneration unit in the network, respectively. Here, F_j^{w} is the flow rate of freshwater to process j; $F_{i,j}$ is the water flow rate from process i to process j; F_j^{RO} is

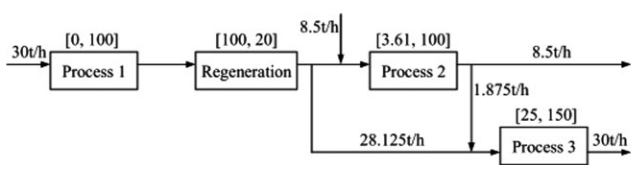

Figure 12. Optimal water network of Example 1 without process decomposition($C_{\mathrm{R}}^{\mathrm{Out}} = 20$ ppm).

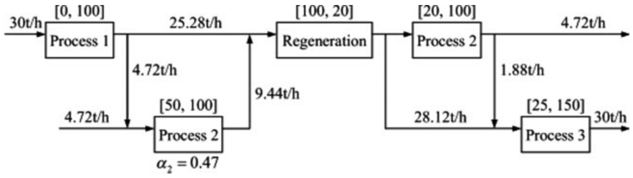

Figure 13. Optimal water network of Example 1 with mass load decomposition($C_R^{Out} = 20$ ppm).

the flow rate of regenerated water to process j; F_j^{D} is the flow rate of water discharged from process j to the end of pipe treatment; $F_{j,k}$ is the water flow rate from process j to process k; F_j^{RI} is the water flow rate from process j to the regeneration unit. The expression $y_{R,j} + y_{j,R} \le 1$ indicates that the connection from process j to the regeneration unit ($y_{j,R}$) and that from the regeneration unit to process j ($y_{R,j}$) cannot coexist. It is noticed that water loss is ignored.

Mathematical Modeling

As previously mentioned, sequential optimization is employed in this article to synthesize the optimal regeneration reuse water network. "Optimal" here corresponds to the network with minimum freshwater consumption, minimum regenerated water flow rate, and minimum contaminant regeneration load. Note that, the "Optimal" only means "near-optimal" because the true optimal can be obtained by simultaneous optimization considering all possible alternatives. In the following, based on the superstructure, freshwater consumption, regenerated water flow rate, and contaminant regeneration load are minimized step by step at certain postregeneration concentrations. As mentioned in the superstructure construction, each water-using process in a system is split into two independent subprocesses. The limiting water data of the subprocesses can be calculated by expressions (1) or (2).

Minimizing freshwater consumption

$$\text{MP1} : \text{Min} \sum_{j \in Q} F_j^{w} \tag{3}$$

s.t.

$$F_j^{w} + \sum_{\substack{i \in Q \\ i \neq j}} F_{i,j} + F_j^{RO} = F_j^{D} + \sum_{\substack{k \in Q \\ k \neq j}} F_{j,k} + F_j^{RI} \quad j \in Q \tag{4}$$

$$\sum_{\substack{i \in Q \\ i \neq j}} (F_{i,j} \cdot C_i^{Out}) + F_j^{RO} \cdot C_R^{Out} = \left(F_j^{W} + \sum_{\substack{i \in Q \\ i \neq j}} F_{i,j} + F_j^{RO} \right) \cdot C_j^{In} \quad j \in Q \tag{5}$$

$$\begin{cases} \left(F_t^{W} + \sum_{\substack{i \in Q \\ i \neq t}} F_{i,t} + F_t^{RO} \right) \cdot C_t^{In} + M_t * \alpha_t \\ = \left(F_t^{W} + \sum_{\substack{i \in Q \\ i \neq t}} F_{i,t} + F_t^{RO} \right) \cdot C_t^{Out} \\ \left(F_{n+t}^{W} + \sum_{\substack{i \in Q \\ i \neq n+t}} F_{i,n+t} + F_{n+t}^{RO} \right) \cdot C_{n+t}^{In} + M_t * (1 - \alpha_t) \\ = \left(F_{n+t}^{W} + \sum_{\substack{i \in Q \\ i \neq n+t}} F_{i,n+t} + F_{n+t}^{RO} \right) \cdot C_{n+t}^{Out} \end{cases} \quad t \in P \tag{6}$$

$$0 \le \alpha_t \le 1 \tag{7}$$

$$\begin{cases} C_t^{In} \le C_t^{In,Max} \\ C_t^{Out} \le C_t^{Out,Max} \\ C_{n+t}^{In} \le C_t^{In,Max} \\ C_{n+t}^{Out} \le C_t^{Out,Max} \end{cases} \quad t \in P \tag{8}$$

or

$$\begin{cases} C_t^{In} \le C_t^{In,Max} \\ C_t^{Out} \le C_t^{I} \\ C_{n+t}^{In} \le C_t^{I} \\ C_{n+t}^{Out} \le C_t^{Out,Max} \\ C_t^{I} = C_t^{In,Max} + \alpha_t \times (C_t^{Out,Max} - C_t^{In,Max}) \end{cases} \quad t \in P \tag{9}$$

$$\sum_{j \in Q} F_j^{RO} = \sum_{j \in Q} F_j^{RI} \tag{10}$$

$$\sum_{j \in Q} (F_j^{RI} * C_j^{Out}) = \sum_{j \in Q} (F_j^{RI} * C_R^{In}) \tag{11}$$

$$C_R^{Out} = c \tag{12}$$

$$\sum_{j \in Q} F_j^{W} \ge \sum_{j \in Q} F_j^{RI} \tag{13}$$

$$\left(F_t^{W} + \sum_{\substack{i \in Q \\ i \neq t}} F_{i,t} + F_t^{RO} \right) - \alpha_t * U \le 0 \quad t \in P \tag{14}$$

$$\left(F_{n+t}^{W} + \sum_{\substack{i \in Q \\ i \neq n+t}} F_{i,n+t} + F_{n+t}^{RO} \right) - (1 - \alpha_t) * U \le 0 \quad t \in P \tag{15}$$

Table 2. Results of Mathematical Programming Versus Targets from Graphical Method for Example 1

Comparison		F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	C_R^{Out}/ppm	M_R^{Min}/kg h^{-1}	α_t
Graphical method		34.72	34.72	100	20	2.78	Nil
Mathematical Programming	No process decomposition	38.5	30	100	20	2.4	0 or 1
	Mass load decomposition	34.72	34.72	100	20	2.78	$\alpha_2 = 0.47$
	Concentration decomposition	35.67	35.67	95.20	20	2.68	$\alpha_2 = 0.4$

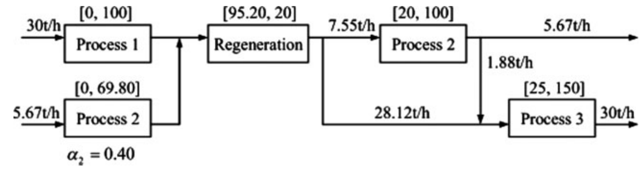

Figure 14. Optimal water network of Example 1 with concentration decomposition($C_R^{Out} = 20$ ppm).

$$F_{i,j} - U^* y_{i,j} \leq 0 \qquad i,j \in Q \tag{16}$$

$$F_j^{RO} - U^* y_{R,j} \leq 0 \qquad i,j \in Q \tag{17}$$

$$F_j^{RI} - U^* y_{j,R} \leq 0 \qquad j \in Q \tag{18}$$

$$y_{R,j} + y_{j,R} \leq 1 \qquad j \in Q \tag{19}$$

$$y_{R,j} \geq y_{i,j} + y_{R,i} - 1 \qquad j \in Q \tag{20}$$

Equation 4 is the flow balance over process j, with the mixer and splitter being inside the balance boundaries. Equation 5 is the mass balance of contaminant s for the mixer node of process j. Equation 6 shows the mass balance of contaminant s for mass transfer in process j. The contaminant mass load of the original process is removed by both two subprocesses and α_t describes how it distributes in subprocesses. As confined in Eq. 7, the value of α_t falls into [0, 1]. The concentration constraints of subprocesses vary with the splitting schemes. Equation 8 gives the constraints for mass load decomposition, and Eq. 9 is those in the case of concentration decomposition. According to the practical situation, one of them will be utilized for each process. Equations 10 and 11 describe the mass balance of regenerated water and mass balance of contaminant for the mixer node before the regeneration unit, respectively. Equation 12 gives a certain postregeneration concentration for the contaminant. In Eq. 13, the flow rate of freshwater is greater than or equal to that of regenerated water. It is the flow rate constraint condition for regeneration reuse that the flow rate of regenerated water never exceeds that of freshwater. Equation 14 ensures that the inlet and outlet flows of subprocess t are equal to 0 when $\alpha_t = 0$, and Eq. 15 ensures that those of subprocess $n+t$ are equal to 0 when $\alpha_t = 1$. U here is a constant, which is greater than any water flow rate between processes. $y_{i,j}$, $y_{R,j}$, and $y_{j,R}$ are all binary variables, and indicate different connections between processes, or between process j and the regeneration unit. Constraints (16)-(18) are introduced to correlate these binary variables with the continuous variables, the corresponding water flow rates. The direct and indirect recycle options can be eliminated by Eqs. 19 and 20, respectively. Equation 19 ensures that a process cannot simultaneously use water from and discharge wastewater to the regeneration unit. When there is a water reuse from process i to process j ($y_{i,j} = 1$), if process i is placed after the regeneration unit ($y_{R,i} = 1$), process j must also be positioned downstream the regeneration unit ($y_{R,j} = 1$) according to Eq. 20; while if process i is at the upstream of the regeneration unit ($y_{R,i} = 0$), there will be no requirements on the location of process j ($y_{R,j} \geq 0$). So Eq. 20 can exclude the indirect recycle options.

To solve the mathematical model above, the limiting water data of water-using processes and whether each water-using process is allowed to split and how to split, should be fully considered for selecting appropriate constraints. In this step, the minimum freshwater consumption of a water system when regeneration reuse is implemented can be obtained, which will be denoted as F_W^{Min} in the following.

Minimizing regenerated water flow rate

Regenerated water flow rate greatly affects the capital cost and operation cost of a regeneration reuse water system. So on the basis of freshwater target, the next step is to optimize regenerated water flow rate and then identify whether total or partial regeneration should be chosen.

$$\text{MP2 : Min} \sum_{j \in Q} F_j^{RO} \tag{21}$$

s.t.

Constraints (4)–(20)

$$\text{and} \sum_{j \in Q} F_j^{w} = F_w^{Min} \tag{22}$$

By solving this model, the minimum regenerated water flow rate F_R^{Min} can be obtained. Moreover, the regeneration scheme can be determined by comparing the regenerated water target F_R^{Min} and the freshwater quantity F_w^{Min}. If the flow rate of regenerated water is equal to that of freshwater,

Table 3. Comparison for the Results of Mathematical Programming with/Without Mass Decomposition Versus Targets From Graphical Method at Different C_R^{Out} for Example 1

	Mathematical Programming Without Process Decomposition				Mathematical Programming with Mass Load Decomposition				Graphical method			
C_R^{Out}/ ppm	F_W^{Min}/ t h^{-1}	F_R^{Min}/ t h^{-1}	$C_R^{In,opt}$/ ppm	M_R^{Min}/ kg h^{-1}	F_W^{Min}/ t h^{-1}	F_R^{Min}/ t h^{-1}	$C_R^{In,opt}$/ ppm	M_R^{Min}/ kg h^{-1}	F_W^{Min}/ t h^{-1}	F_R^{Min}/ t h^{-1}	$C_R^{In,opt}$/ ppm	M_R^{Min}/ kg h^{-1}
10	35.5	30	100	2.7	32.89	32.89	100	2.96	32.89	32.89	100	2.96
20	38.5	30	100	2.4	34.72	34.72	100	2.78	34.72	34.72	100	2.78
25	40	30	100	2.25	35.71	35.71	100	2.68	35.71	35.71	100	2.68
30	41.5	30	100	2.1	38.42	34.40	100	2.70	36.76	36.76	100	2.57
40	44.5	30	100	1.8	42.73	32.95	105.98	2.17	41.25	35.42	100	2.12

Table 4. Results of Mathematical Programming Only with Concentration Decomposition of P3

C_R^{Out}/ppm	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	M_R^{Min}/kg h^{-1}
30	41.5	30	100	2.1
40	44.5	30	100	1.8

total regeneration should be implemented, otherwise partial regeneration is chosen.

Minimizing contaminant regeneration load

Finally, contaminant regeneration load is further minimized to guarantee a lower regenertion cost of regeneration reuse water systems

$$\text{MP3 : Min} \sum_{j \in Q} F_j^{RO} * (C_R^{In} - C_R^{Out}) \tag{23}$$

s.t.

Constraints (4)–(20), (22)

$$\text{and} \sum_{j \in Q} F_j^{RO} = F_R^{Min} \tag{24}$$

The optimal regeneration reuse water network can be finally constructed by solving this programming.

Splitting factor α describes to what extent a water-using process is decomposed. Despite whether and how processes are split, the three mathematical models above are always applicable. Through setting $\alpha_t = 1$ or $\alpha_t = 0$, water-using process t will not be decomposed, while $0 < \alpha_t < 1$ represents process t can be decomposed. If there is no special requirement on process t, just keep $0 \le \alpha_t \le 1$. The optimal splitting factor for each water-using process can be determined by solving the three models in sequence.

Application of mathematical models

Several suggestions are presented here as reference for application of the models above.

(1) In an actual water-using system, there will be distinctive requirements on different water-using processes. Some processes are not allowed to split, while others may be decomposed by contaminant mass load or concentration. Therefore, constraints on concentrations and splitting factors should be correctly selected according to the features of each water-using process.

(2) All the mathematical models above belong to MINLP, which can be solved by commercial software, such as LINGO or GAMS. Because of process decomposition, variables of the models multiply in comparison with the case of no process decomposition. Therefore, it is helpful to set appropriate initial values for several parameters to expedite solving. Commonly, the outlet contaminant concentration of each water-using process is initialized as the limiting outlet concentration.

(3) As a matter of fact, several water-using processes in a system do not need to be decomposed according to their characteristics. The corresponding splitting factor can be directly set to be zero. For instance, if one water-using process has a limiting inlet concentrations equal to the corresponding concentration of freshwater, it can only use freshwater, while processes with limiting inlet concentration higher than regeneration concentration can take wastewater from other processes as sources. Thus process decomposition is not necessary for both of them.

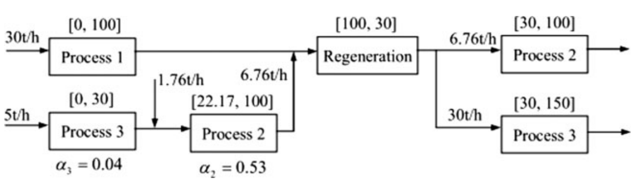

Figure 15. Target water network of Example 1 when C_R^{Out} = 30 ppm.

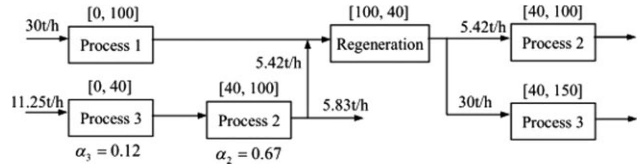

Figure 16. Target water network of Example 1 when C_R^{Out} = 40 ppm.

Case Study

In the following, four examples are employed to show the applicability of the mathematically based methodology proposed in this article. Then by comparing the results of mathematical programming in different cases with the targets from graphical method,[11] the optimal decomposition strategies for single-contaminant systems can be summarized to realize the target regeneration reuse water network. Note that all the MINLP problems in this article are solved by the commercial software package LINGO 8.0. Generally, it cannot guarantee to obtain global optimum solution with the MINLP model. In this article, firstly, the local optimum solver in LINGO 8.0 is utilized to get several local optimal solutions. Secondly, several local optimal solutions are set to the initial value and the global optimum solver in LINGO 8.0 is applied to solve the model. For the cases with single contaminant, once the results are compatible with those obtained from graphical approach, the global optimum solutions are considered to be reached.

Example 1. The single-contaminant water system in Table 1 is revisited here.

The postregeneration concentration is assumed to be 20ppm. If water-using processes are not allowed to split, that is, $\alpha_t = 1$ or $\alpha_t = 0$. By solving MP1, the freshwater target of the system with regeneration reuse can be obtained as 38.5 t/h. In addition, the minimum regenerated water flow rate can be

Table 5. Limiting Process Data for Example 2

Process	$C^{In,Max}$/ppm	$C^{Out,Max}$/ppm	Mass Load/kg h^{-1}
1	0	50	1.25
2	30	50	0.525
3	50	60	0.6
4	60	110	0.75

Table 6. Comparison for the Results of Mathematical Programming With/Without Mass Decomposition Versus Targets From Graphical Method at Different C_R^{Out} for Example 2

	Mathematical Programming Without Process Decomposition				Mathematical Programming With Mass Load Decomposition				Graphical Method			
C_R^{Out}/ppm	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	M_R^{Min}/kg h^{-1}	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	M_R^{Min}/kg h^{-1}	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	M_R^{Min}/kg h^{-1}
10	25	21.88	50	0.875	25	17.5	60	0.875	25	17.5	60	0.875
20	27.08	25	50	0.75	25	21.88	60	0.875	25	21.88	60	0.875
30	30.83	26.25	60	0.787	26.39	26.39	60	0.792	26.39	26.39	60	0.792
40	35.42	25	50	0.25	31.56	24.06	60	0.481	31.56	24.06	60	0.481
50	39.58	0	-	-	35.5	24.5	60	0.245	35.5	24.5	60	0.245

calculated as 30 t/h by solving P2, which is less than the freshwater flow rate (30 t/h < 38.5 t/h), thus partial regeneration is chosen for this water system. After solving MP3, the resultant water network without process decomposition can be synthesized as shown in Figure 12. In the similar way, the optimal targets can be obtained as shown in Table 2 via solving the MP1, MP2, and MP3 with $0 \leq \alpha_t \leq 1$ and concentration constraint (8). Note that the calculated splitting factor for P2 with mass load decomposition is 0.47. As shown in Table 2, the target flow rates of freshwater and regenerated water both are 34.72 t/h. The results are better than those obtained graphically before when splitting factor is 0.5. The optimal regeneration reuse water network with mass load decomposition of processes can also be constructed as shown in Figure 13. Moreover, the optimal targets of concentration decomposition are shown in Table 2 via solving the MP1, MP2, and MP3 with $0 \leq \alpha_t \leq 1$ and concentration constraint (9). In addition, the splitting factor for process 2 with concentration decomposition is calculated as 0.4. As shown in Table 2, the target flow rates of freshwater and regenerated water are the same as 35.72 t/h. Similarly, the results are better than those obtained graphically with splitting factor as 0.5. Figure 14 gives the optimal regeneration reuse water network with concentration decomposition.

The optimal targets of the single contaminant water system with regeneration reuse can also be obtained via the proposed graphical approach,[11] as shown in Table 2. From Table 2, it can be seen that, the results of mathematical programming vary with the decomposition schemes. Without process decomposition, the minimum freshwater consumption of the system is larger than the freshwater target from graphical method (38.5 t/h > 34.72 t/h). When process decomposition is considered, mass load decomposition ensures that the resultant network totally reaches the targets from graphical method, while concentration decomposition fails. That is to say, mass load decomposition excels in saving freshwater to certain extent.

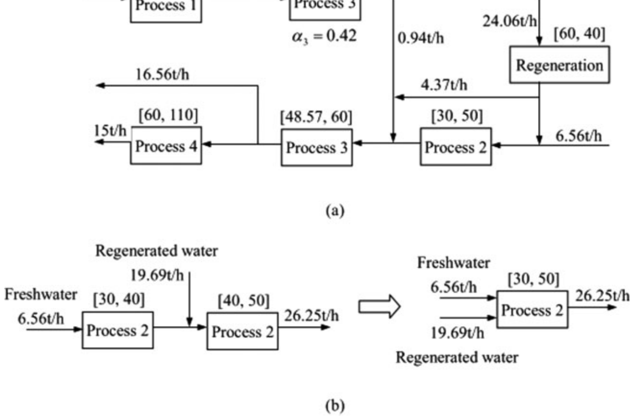

Figure 17. Target water network of Example 2 when $C_R^{Out} = 40$ ppm.

At the postregeneration concentration of 20 ppm, the target regeneration reuse water network can be realized by mass load decomposition of processes. So how about the results in case of a higher or a lower postregeneration concentration? Table 3 gives the optimized results of mathematical programming with or without mass load decomposition schemes at a series of postregeneration concentrations versus the corresponding targets determined via the proposed graphical approach.[11] Through comparison, it can be concluded that, without process decomposition, the resultant network at any postregeneration concentration cannot meet the targets. If the postregeneration concentration is less than or equal to the second lowest limiting inlet concentration of the system (e.g., 25 ppm for Example 1), merely mass load decomposition can implement the target network. However, if the postregeneration concentration is higher, such as 30 ppm and 40 ppm in Table 3, mass load decomposition seems to be not enough. The graphical analysis in the previous sections may reveal several tips to reach the optimal results. When the postregeneration concentration is higher than the second lowest limiting inlet concentration of the system (i.e., 25 ppm for Example 1), the concentration decomposition of certain water-using process is of benefit to freshwater reduction. Note that, the postregeneration concentration should locate in the limiting concentration interval of such a process (i.e., P3 for Example 1). The process with zero limiting inlet

Table 7. Limiting Process Data for Example 3

Process	$C^{In,Max}$/ppm	$C^{Out,Max}$/ppm	Mass Load /kg h^{-1}
1	25	80	2.0
2	25	90	2.88
3	25	200	4.0
4	50	100	3.0
5	50	800	30.0
6	400	800	5.0
7	400	600	2.0
8	0	100	1.0
9	50	300	20.0
10	150	300	6.5

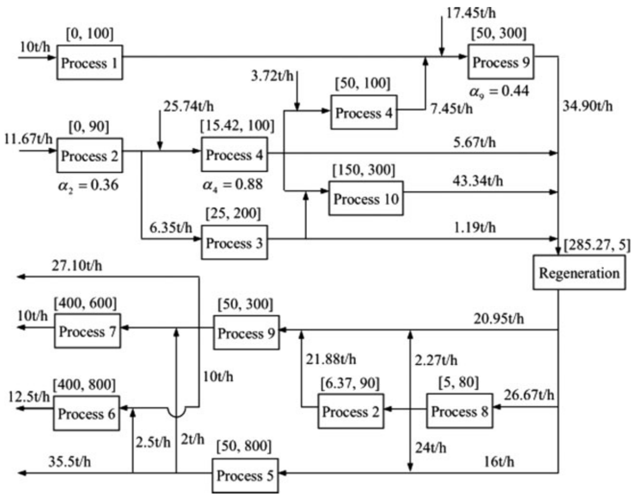

Figure 18. Target water network of Example 3.

concentration (i.e., P1 for Example 1) is excluded because concentration decomposition of it will not reduce freshwater.

Here, take the postregeneration concentration as the interim concentration and only consider concentration decomposition of P3 when the postregeneration concentration is set to be 30 ppm or 40 ppm. The optimized results are shown in Table 4. Apparently they are still not equal to the targets from graphical method.[11] Then further resort to mass load decomposition. All the water-using processes or subprocesses after concentration decomposition are now taken as a new system and the process with limiting inlet concentration higher than the postregeneration concentration is considered to be decomposed. In this way, all the parameters will be in compliance with the targets via the proposed graphical approach[11] as shown in Table 3. Figure 15 shows the target regeneration reuse water network at the postregeneration concentration of 30 ppm, when total regeneration should be installed, and Figure 16 is the resultant network at 40ppm, when partial regeneration is the desirable choice.

Therefore, for this example system, when the postregeneration concentration is higher than the second lowest limiting inlet concentration of the system, the combination of mass load and concentration decomposition of processes realizes the target regeneration reuse water network, whatever regeneration mode (total or partial) is utilized.

Example 2. Consider a water network design problem consisting of four water-using processes and a single contaminant. The limiting process data are shown in Table 5.

By selecting the corresponding concentration constraints and solving the three mathematical models step by step, the optimized results with and without process decomposition at different postregeneration concentrations can be calculated, as listed in Table 6. In addition, the targets obtained via the proposed graphical approach[11] are also shown in Table 6, from which it can be seen that, at most postregeneration concentrations (except for 30 ppm), partial regeneration is the optimal choice for the system. Similar to Example 1, Table 6 indicates that without process decomposition the targets cannot be achieved at any postregeneration concentration. However, different from Example 1, merely by mass load decomposition of processes, all the optimized results accord with the targets from graphical method, even when the postregeneration concentration is higher than the second lowest limiting inlet concentration of the system (30 ppm). Take $C_R^{Out} = 40$ppm for example, Figure 17a shows the target regeneration reuse water network. Obviously concentration decomposition is not utilized here, yet this is actually a special case, which can be illustrated by Figure 17b. In Figure 17b, water-using process 2, the limiting concentration interval of which contains the postregeneration concentration (30 ppm $<$ 40 ppm $<$ 50 ppm), is in fact split into two subprocesses originally. It is simply that the subprocesses are series-arranged and then can be automatically combined together without any freshwater penalty.

According to the results of the examples above, several heuristic rules on optimizing and designing single-contaminant regeneration reuse water networks can be summarized as follows.

(1) Process decomposition is resorted to further reduce the flow rates of freshwater and regenerated water, and contaminant regeneration load when synthesizing regeneration reuse water networks.

(2) When the postregeneration concentration is less than or equal to the second lowest limiting inlet concentration of a system, mass load decomposition of processes is only needed. While if postregeneration concentration is higher, first conduct concentration decomposition on the process, the limiting concentration interval of which passes through the postregeneration concentration. If the results do not fulfill the targets, on the basis of concentration decomposition, consider mass load composition next.

(3) In the case of partial regeneration reuse, the limiting freshwater consumption of a water system can be easily identified.[11] According to the feature of partial regeneration reuse, the optimization procedures can be simplified to some extent. If the optimizing result of the first model (MP1) is greater than the limiting freshwater consumption, total regeneration reuse has to be utilized, that is, the flow rate of regenerated water is equal to that of freshwater. So the second model (MP2) for minimizing the regenerated flow rate can be skipped and the third model (MP3) can be directly carried out. While if the result of the first model (MP1) is equal to the limiting freshwater consumption, partial regeneration will be chosen, then the regenerated water flow rate, contaminant regeneration load should be routinely optimized in sequence.

According to these experience-based rules, the way to implement the target regeneration reuse water network is

Table 8. Results in this Article Versus Results in Literature Sources for Example 3

Comparison	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	C_R^{Out}/ppm	M_R^{Min}/kg h^{-1}
Bagajewicz and Savelski[20]	91.12	79.6	300	5	23.48
In this article	85.10	85.10	285.3	5	23.85
Graphical method	85.10	85.10	285.3	5	23.85

Table 9. Limiting Process Data for Example 4

Process	$C^{In,Max}$/ppm	$C^{Out,Max}$/ppm	Mass Load /kg h^{-1}
1	0	250	6.25
2	50	300	15.0
3	150	400	7.5
4	300	500	14.0

clarified. In the following, two examples from the literature sources are employed to demonstrate the feasibility of the rules.

Example 3. Consider a single-contaminant water system consisting of 10 water-using processes and a single contaminant and one regeneration unit with the limiting process data shown in Table 7.[20] The postregeneration concentration is given as 5 ppm.

In the literature source,[20] a MILP model is developed to synthesize the regeneration reuse water network with minimum freshwater usage in the case of no process decomposition. Here process decomposition is utilized to further reduce the freshwater consumption and wastewater generation of the system. Since the postregeneration concentration is lower than the second lowest limiting inlet concentration of the system (5 ppm $<$ 25 ppm), only mass load decomposition will be enough. Based on the concentration constraint (8) and $0 \le \alpha_t \le 1$ as well as the limiting data in Table 7, the minimum freshwater consumption can be obtained as 85.10 t/h via solving MP1. Since at the postregeneration concentration of 5 ppm, the limiting freshwater consumption of the system is 10 t/h, which is lower than 85.10 t/h, total regeneration can be directly identified without optimization of the second step. In other words, the minimum regenerated water flow rate is also 85.10 t/h. According the second rule, the second model (MP2) is skipped. Then by solving MP3, the target regeneration reuse water network can be constructed, as is shown in Figure 18. Table 8 lists the results of this article, those of the literature and the targets determined by graphical method.[11] It can be seen that, three processes (P2, P4 and P9) are split via mass load decomposition and the corresponding splitting factors are 0.36, 0.88, and 0.44, respectively. The freshwater consumption of the system is reduced from 91.12 t/h to 85.10 t/h, which conforms to the targets via the proposed graphical approach.[11]

Example 4. This is a single-contaminant system with four water-using processes, which has been considered both

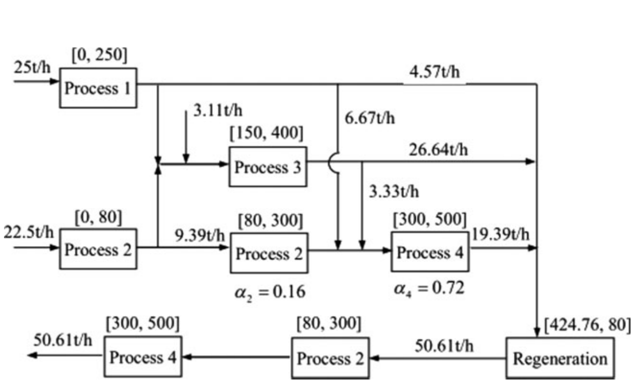

Figure 19. Target water network of Example 4 when $C_R^{Out} = 80$ ppm.

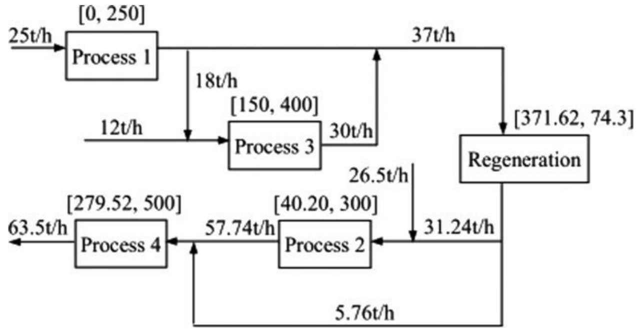

Figure 20. Optimal water network of Example 4 without process decomposition ($C_R^{Out} = 74.3$ ppm).

by Castro et al.[4] and Xu et al.[26] Table 9 shows the limiting process data of the system. The objective here is to design a regeneration reuse network that features minimum freshwater consumption, minimum regenerated water flow rate and minimum contaminant regeneration load.

Following the literature sources,[4,26] the postregeneration concentration is set to be 80 ppm when process decomposition is considered. In the case of no process decomposition, the postregeneration concentration is set to be 74.3 ppm as in the literature[4,26] for comparison. Before design, we first briefly analyze the system to make some preparation for mathematical models construction. Firstly, to meet the design requirements for this problem, water-using processes should be split. Then, since the postregeneration concentration, 80 ppm, is higher than the second lowest limiting inlet concentration of the system, 50 ppm, concentration decomposition is considered first. Apparently, the postregeneration concentration falls into the limiting concentration interval of P2 (50 ppm $<$ 80 ppm $<$ 300 ppm), thus concentration decomposition is performed on P2 with 80 ppm as the interim concentration. Next, take all the processes after concentration decomposition as a new system and further conduct mass load decomposition. P1 with the limiting inlet concentration equal to 0 need not to be split since freshwater is the only source. While for other processes, mass load decomposition should be initially supposed. Last, according to the analysis on splitting scheme, the mathematical models can be built and solved. As shown in Figure 19, P2 is firstly split by concentration interval with 80 ppm as the interim concentration and then split by mass load with splitting factor as 0.16, while P4 is only conducted mass load decomposition with splitting factor as 0.72. Additionally, for comparison with the results in the literature sources, Figure 20 gives the optimal regeneration reuse network without process decomposition and Figure 21 shows the situation when only mass load decomposition is considered.

Table 10 compares the optimizing results in this article with those in the literature sources. From Table 10, it can be seen that, in the case of no process decomposition, all the optimizing results are same, although the resultant networks are slightly different. If processes are split by mass load, compared with the results of Castro et al.,[4] the freshwater consumption decreases from 60.2 t/h to 57.328 t/h. While in comparison with the results of Xu et al.,[26] the flow rates of both freshwater and regenerated water are the same.

Table 10. **Results in this article Versus Results in the Literature Sources for Example 4**

	Comparison	F_W^{Min}/t h^{-1}	F_R^{Min}/t h^{-1}	$C_R^{In,opt}$/ppm	C_R^{Out}/ppm	M_R^{Min}/kg h^{-1}
Castro et al[4]	No process decomposition	63.5	37	371.6	74.3	11.0
	Mass load decomposition	60.2	39.5	400	80	12.65
Xu et al[26]	No process decomposition	63.5	37	371.6	74.3	11.0
	Mass load decomposition	57.328	43.5	481.15	80	17.45
	Mass load and concentration decomposition	50.596	50.596	424.94	80	17.45
In this article	No process decomposition	63.5	37	371.6	74.3	11.0
	Mass load decomposition	57.328	43.5	472.77	80	17.09
	Mass load and concentration decomposition	50.606	50.606	424.76	80	17.45
Graphical method		50.595	50.595	424.94	80	17.45

However, the optimal regeneration concentration (472.77 ppm) is lower than that (481.15 ppm) in Xu et al.[26] and the calculated contaminant regeneration load (17.09 kg h^{-1}) is also less than that (17.45 kg h^{-1}) in Xu et al.,[26] which would cause a lower regeneration cost. If mass load decomposition and concentration decomposition are combined, the results of our method are consistent with those of Xu et al.[26] and the targets obtained via the proposed graphical approach[11] (The tiny differences on flow rates and regeneration concentration are tolerated by calculating errors), yet the resultant water networks are different.

Conclusions

Process decomposition, including mass load decomposition and concentration decomposition, lowers the requirements of water-using processes on water quantity or quality, thus is an effective way to reduce the freshwater usage and wastewater discharge of a regeneration reuse water system. The sequential-optimization-based models developed in this article take process decomposition into account. They are capable of designing single-contaminant regeneration reuse water networks with different decomposition schemes. A graphically based method[11] delivers the targets of a single-contaminant regeneration reuse water system, while the decomposition strategies summarized by several examples in this article can realize the corresponding network. The heuristic rules for process decomposition are summarized and then are combined into mathematical programming. The approach in this article can be viewed as mathematical programming combined graphical analysis. Moreover, postregeneration concentration is an influential factor on decomposition strategies. When the postregeneration concentration is lower than or equal to the second lowest limiting inlet concentration of a system, only mass load decomposition needs to be considered. While if the postregeneration concentration is higher, mass load decomposition and concentration decomposition should be combined.

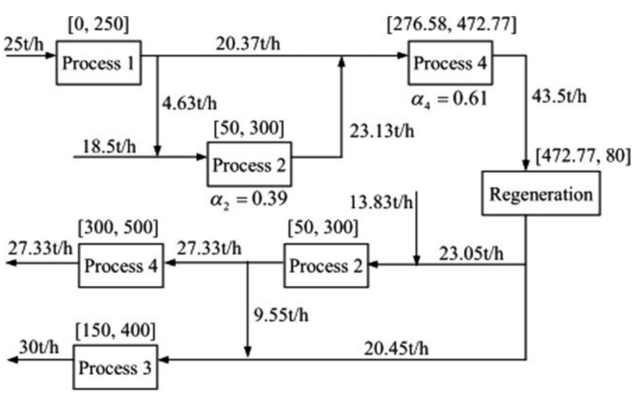

Figure 21. Optimal water network of Example 4 with mass load decomposition ($C_R^{Out} = 80$ ppm).

Note that process decomposition reduces the freshwater usage and wastewater discharge, thus is considered in regeneration reuse water systems. However, from the industry application point of view, decomposition complicates network structure, and sometimes is even unfeasible. And in terms of model solving, decomposition multiplies optimizing variables and increases model dimensions, which incur a series of solving difficulties. Furthermore, process decomposition, which is generally considered in new design, is hard to be applied to retrofit problems. Therefore, when process decomposition is considered in a practical water system, several factors, such as freshwater consumption (wastewater generation), network structure and decomposition feasibility, should be overall weighted to make a reasonable choice.

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Notation

α = splitting factor
$C_i^{in,Max}$ = limiting inlet concentration for process i, ppm
$C_i^{Out,Max}$ = limiting outlet concentration for process i, ppm
C_R^{Out} = the inlet concentration for the regeneration unit, ppm
C_R^{Out} = postregeneration concentration for the regeneration unit, ppm
C^I = the interim concentration for the concentration decomposition, ppm
F_j^w = flow rate of freshwater allocated to process j, t/h
$F_{i,j}$ = water flow rate of process i allocated to process j, t/h
F_j^{RI} = water flow rate from process j to the regeneration unit, t/h
F_j^{RO} = flow rate of regenerated water allocated to process j, t/h
F_j^D = flow rate of water discharged from process j to the end of pipe treatment, t/h
F_w^{Min} = the targeted minimum freshwater flow rate, t/h
F_R^{Min} = the targeted minimum flow rate of regenerated flow rate, t/h
M = contaminant mass load, kg/h
M_t = contaminant mass load of process t, kg/h
MP = mathematical programming model
P = set of water-using processes before decomposition, $P\{1, 2, 3, \ldots t \ldots, n\}$
Q = set of water-using processes after decomposition, $Q\{1, 2, 3, \ldots j \ldots, 2n\}$
$y_{i,j}$ = binary variable related to the connection from process i to process j
$y_{j,R}$ = binary variable related to the connection from process j to the regeneration unit

y_{Rj} = binary variable related to the connection from the regeneration unit to process j

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