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A Heuristic Design Procedure for Water-Using Networks with Multiple Contaminants

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On the analogy of the water-using networks with single contaminant, we will introduce new methodology concepts: the concentration potentials of the demand streams and those of the source streams in the water-using systems with multiple contaminants, based on the overall allocation possibility of the source streams to the demand streams. In the design procedure, the performing order of the processes is determined by the inlet concentration potentials of the processes. The processes with the lowest inlet concentration potential will be performed first. When satisfying the inlet stream of the process being performed, the source with the largest quasi-allocation amount, which is defined in this article, will be used first. A few literature examples are investigated to show the method proposed. The results show that the method proposed in this work is very simple and the freshwater consumptions of the designs obtained are very close to the minimum freshwater targets.
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Introduction

Wastewater minimization has received much attention because the increases in the costs of freshwater and wastewater effluent treatment and the introduction of strict environmental regulations. In the following discussion, we will mainly discuss the work which dealt with the water systems with multiple contaminants. Takama et al.[1] used mathematical programming to optimize the superstructure of the water-using systems. El-Halwagi and Manousiouthakis[2] addressed the more general problem of mass exchange networks by introducing the composite curves to denote mass exchange operations. Wang and Smith[3] investigated the problem of wastewater minimization by maximum reuse and regeneration reuse with a graphical approach. Doyle and Smith[4] studied the minimum freshwater requirement targets of the water networks with multiple contaminants by combining linear programming (LP) and nonlinear programming (NLP) optimization in an iterative procedure. Wang and Smith[5] and Kuo and Smith[6] proposed manual approaches for the design of distributed effluent treatment systems. Galan and Grossmann[7] introduced a superstructure optimization approach for the design of distributed effluent treatment systems. Kuo and Smith[8] presented a numerical method for design of the water-using systems involving regeneration reuse. Alva-Argáez et al.[9] presented an approach which combines insights from water pinch with mathematical programming. The approach can be applied to the mass exchanger networks and wastewater minimization problems. Its purpose is the development of targeting models at a conceptual stage. Gunaratnam et al.[10] presented an automated design method for total water systems by using a mixed-integer nonlinear programming approach.

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Feng and Seider[11] proposed a design method by introducing single or multiple internal water mains, which are reservoirs at a uniform concentration of contaminants in the water-using networks. Wang et al.[12] proposed a design procedure for the water-using networks with a single internal water main. Wang et al. addressed that by introducing a single internal water main, freshwater consumption can be reduced sharply. However, freshwater consumption obtained by Wang et al.[12] is much higher than the target value. Zheng et al.[13] proposed a general methodology for the optimal design of the water-using networks with multiple internal water mains by using a superstructure and a mixed-integer nonlinear programming (MINLP) strategy. The most effective designs obtained by the method of Zheng et al.[13] exceed the results of Wang et al.[12] However, freshwater consumptions are still higher than the target values. Alva-Argáez et al.[14] proposed a systematic methodology that empowers conceptual engineering and water-pinch with mathematical programming methods. The method focused on petroleum refineries and tried to explain trade-offs and savings between freshwater costs, wastewater treatment, piping costs, and environmental constraints on the discharge. Karuppiah and Grossmann[15] addressed the problem of optimal synthesis of an integrated water system, in which water-using processes and water treatment operations are combined into a single network. In this way, the total cost of obtaining freshwater in the water-using operations and treating wastewater is globally minimized. A superstructure is proposed in which all feasible design options for water treatment, reuse, and recycle are included. This superstructure is solved to global optimality as a nonconvex NLP problem. Bagajewicz et al.[16] presented necessary conditions of optimality for multiple contaminants water allocation systems in refineries and process plants. They extended the necessary conditions of optimality for single contaminant systems proved by Savelski and Bagajewicz.[17] They showed that at least one contaminant should reach the maximum concentration at the outlet of a freshwater user process.

From the above discussion, it can be seen that both graphical approaches and numerical optimization programming methods were used to solve the problems of the design and targeting of the water systems with multiple contaminants.

Generally speaking, the targeting and design of a water network with multiple contaminants are much more difficult than that of a water network with single contaminant. For a water network with single contaminant, the demand (inlet) streams and source (outlet) streams can be arranged in ascending order of their concentrations, respectively. Then, the demand streams can be satisfied by the source streams in turn. The minimum freshwater requirement target can be obtained graphically or numerically.[3,18–21] The optimal design can also be obtained easily.[3,22] However, for a water network of multiple contaminants, it is difficult to determine the concentration order of the demand streams and that of the source streams.

In this article, we will investigate the design of the fixed-mass-load water-using networks of multiple contaminants. We will introduce new methodology concepts to determine the concentration order of the demand streams and that of the source streams based on the overall possibility of the allocation of the source streams to the demand streams. A heuristic design procedure will be proposed on the analogy of the design procedure of the water-using networks of single contaminant. A few literature examples will be investigated to show the design procedure proposed.

Basic Concepts: The Concentration Potentials of the Source and Demand Streams

In a water-using system, freshwater consumption can be reduced by maximum reuse of the source streams for the demand streams. Because of complexity of the problem, many researchers used NLP, MINLP, or other optimization approaches to obtain the optimal design for a system with multiple contaminants. In this article, on the analogy of design of the water-using networks with single contaminant, we will propose new methodology concepts which can be used to develop a simple method to solve the design problem for the water-using networks with multiple contaminants involving reuse of the source streams to the demand streams.

As discussed earlier, it is sometimes difficult to determine the concentration order of the demand streams and that of the source streams for a water-using system of multiple contaminants. Let us use an example to show this by considering the limiting data in Table 1 of a water-using network taken from Wang et al.[12] From Table 1, it can be seen that the limiting inlet concentrations of process 3, in ppm, (40, 60, 20), are lower than those of process 5, (110, 135, 60), and those of process 6, (200, 170, 150). However, it is difficult to tell if the limiting inlet concentrations of process 3 are lower than those of process 4, (30, 40, 70), because the limiting inlet concentrations of contaminants *A* and *B* in process 3 are higher than those in process 4, but the limiting inlet

Table 1. Limiting Process Data for Example 1 from Wang et al.[12]

Process	Contaminant	$F^{\max}$ (t/h)	$C^{\max,\text{in}}$ (ppm)	$C^{\max,\text{out}}$ (ppm)
1	A	30	0	100
	B		0	90
	C		0	50
2	A	16	0	50
	B		0	70
	C		0	70
3	A	75	40	150
	B		60	80
	C		20	70
4	A	21	30	160
	B		40	100
	C		70	90
5	A	29	110	210
	B		135	200
	C		60	120
6	A	40	200	350
	B		170	400
	C		150	210
7	A	61	100	300
	B		75	290
	C		20	170
8	A	57	90	210
	B		50	170
	C		34	100

concentration of contaminant C in process 3 is lower than that in process 4. It is also difficult to tell if the limiting inlet concentrations of process 8, (90, 50, 34) are higher than those of process 7 (100, 75, 20). The situation discussed earlier can be found in many other systems.

For a water-using network of single contaminant, it is clear that the lower the concentration of a demand stream, the lower the possibility for it to reuse the source streams. Similarly, the lower the concentration of a source stream, the higher the possibility for it to be reused by the demand streams. The facts mentioned above should be true as well for a water-using network of multiple contaminants. Although it is difficult to determine the concentration order of the streams of a multiple contaminants network in conventional way, it is possible to determine the overall possibility of each demand stream to reuse the source streams, and the overall possibility of each source stream to be reused by the demand streams. It is reasonable to take the order of the overall possibilities of the demand streams to reuse the source streams as the concentration order of the demand streams, and similarly, to take the order of the overall possibilities of the source streams to be reused by the demand streams as the reverse order of the concentrations of the source streams.

In design of the water-using networks, one of the important objectives is to reduce freshwater consumption as much as possible. For this purpose, for a water-using network of single contaminant, the outlet concentration of a process which needs freshwater should reach the maximum. For a water-using network of multiple contaminants, Bagajewicz et al.[16] addressed that at least one contaminant should reach the maximum concentration at the outlet of a freshwater user process. On the other hand, freshwater consumption can be reduced by reusing the source (outlet) streams as much as possible. For this purpose, at least one contaminant should reach the maximum concentration at the inlet of a freshwater user process in most cases. In this article, we want to obtain indicators to determine the concentration order of the streams. Then, we will assume that for all the demand streams (both freshwater user processes and nonfreshwater user processes), at least one contaminant should reach the maximum concentrations.

For convenience, we denote the allocation of source stream S_i to demand stream D_j as (S_i, D_j). Let us consider unit amount (say, 1 ton) of demand D_j is satisfied by source S_i. As discussed earlier, when D_j is satisfied, the concentration(s) of at least one contaminant will reach the limiting value(s):

$$C_{Dj,k} \leq C_{Dj,k}^{\lim} \quad (k = 1, 2, \ldots, \mathrm{NC}) \tag{1}$$

where $C_{Dj,k}$ is the concentration of contaminant k in demand D_j, $C_{Dj,k}^{\lim}$ is the limiting concentration of contaminant k in demand D_j, and NC is the number of contaminants.

When S_i is allocated to 1 ton of D_j, the contaminant(s), whose concentration reaching the limiting value first, will limit the allocation, and will be called as the reuse key contaminant(s) (RKCs) for (S_i, D_j). Let $R_{i,j}$ be the maximum quasi-allocation amount of S_i for 1 ton of D_j. For the RKC, the limiting mass load in 1 ton of D_j is assumed to be equal to the mass load allocated from S_i:

$$1 \times C_{Dj,\mathrm{RKC}}^{\lim} = R_{i,j} \times C_{Si,\mathrm{RKC}} \tag{2}$$

where $C_{Si,RKC}$ is the concentration of the *RKC* in S_i. Then, from Eqs. 1 and 2, we have

$$R_{i,j} = \frac{C_{Dj,\mathrm{RKC}}^{\lim}}{C_{Si,\mathrm{RKC}}} = \min_{k=1,2\cdots,\mathrm{NC}} \left(\frac{C_{Dj,k}^{\lim}}{C_{Si,k}} \right) \tag{3}$$

where $C_{Si,k}$ is the concentration of contaminant k in source S_i.

From Eq. 3, if $C_{Dj,\mathrm{RKC}}^{\lim} < C_{Si,\mathrm{RKC}}$, then $R_{i,j} < 1$. In this situation, freshwater is required. The $R_{i,j}$ value could be the real allocation amount of (S_i, D_j), if the amount of the source is sufficient.

If $C_{Dj,\mathrm{RKC}}^{\lim} = C_{Si,\mathrm{RKC}}$, then $R_{i,j} = 1$. In this situation, freshwater is not required. The $R_{i,j}$ value could also be the real allocation amount of (S_i, D_j), if the amount of the source is sufficient.

If $C_{Dj,\mathrm{RKC}}^{\lim} > C_{Si,\mathrm{RKC}}$, then $R_{i,j} > 1$. In this situation, freshwater is not required. The maximum quasi-allocation amount will be larger than the limiting flowrate of D_j. This is one of the reasons that we call $R_{i,j}$ as the maximum *quasi*-allocation amount. In this situation, although the value of $R_{i,j}$ cannot be the real allocation amount of (S_i, D_j), it still reflects the possibility of S_i to be reused by 1 ton of D_j.

From the above discussion, it can be seen that $R_{i,j}$ can reflect the possibility of 1 ton of D_j to reuse S_i. We define the ***concentration potential*** of demand D_j, CPD(D_j), as the sum of the $R_{i,j}$ values for all the source streams:

$$\mathrm{CPD}(D_j) = \sum_{i=1}^{\mathrm{NS}} R_{i,j} = \sum_{i=1}^{\mathrm{NS}} \min_{k=1,2,\cdots,\ \mathrm{NC}} \left[\frac{C_{Dj,k}^{\lim}}{C_{Si,k}} \right] \quad (i \neq j) \tag{4}$$

where $i \neq j$ because for a fixed-mass-load water-using system, when only reuse is considered, it is meaningless to recycle a water stream to the process where it is produced, and NS is the number of the sources.

From the above discussion, it can be seen that the value of CPD(D_j) depends on the contaminant concentrations only. The value of CPD(D_j) reflects the overall possibility of demand D_j to reuse the source streams. The lower the value of CPD(D_j), the lower the overall possibility for demand D_j to reuse the source streams, and the lower the concentration of the demand stream. This agrees with the features of the concentrations of a water-using network of single contaminant.

Similarly, the mass load of 1 ton of source S_i can be reused to satisfy $1/R_{i,j}$ tons of D_j. The sum of the values of $1/R_{i,j}$ for all the demand streams can reflect the overall possibility of the demands to reuse S_i:

$$\mathrm{SF}(S_i) = \sum_{j=1}^{\mathrm{ND}} \frac{1}{R_{i,j}} \tag{5}$$

where ND is the number of the demand streams, and the reason for $i \neq j$ is the same as discussed earlier.

Although the value of SF(S_i) can reflect the overall possibility of the demands to reuse S_i, it might encounter numerical difficulties when $R_{i,j}$ is very small, especially when the

Table 2. Concentration Potentials of Example 1

D_j	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
$CPD(D_j)$	0	0	1.48	1.54	4.52	9.00	1.66	2.45
Order	1	2	3	4	7	8	5	6
S_i	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8
$CPS(S_i)$	0.22	0.22	0.33	0.37	0.63	1.46	0.75	0.50
Order	1	2	3	4	6	8	7	5

value of $R_{i,j}$ is zero. To avoid the numerical difficulties, an alternative indicator will be introduced. As discussed earlier, the value of $R_{i,j}$ can reflect the possibility of S_i to be reused by 1 ton of D_j. Therefore, we will calculate the overall possibility of S_i to be reused by the demand streams as follows:

$$\mathrm{CF}(S_i) = \sum_{j=1}^{\mathrm{ND}} R_{i,j} \quad (i \neq j) \tag{6}$$

where the reason for $i \neq j$ is the same as discussed earlier.

The larger the value of $\mathrm{CF}(S_i)$, the stronger the overall possibility for S_i to be reused by the demand streams. To be consistent with the $\mathrm{CPD}(D_j)$, we define the reciprocal of $\mathrm{CF}(S_i)$ as the ***concentration potential*** of source stream S_i:

$$\mathrm{CPS}(S_i) = \frac{1}{\mathrm{CF}(S_i)} = \frac{1}{\sum_{j=1}^{\mathrm{ND}} R_{i,j}} = \frac{1}{\sum_{j=1}^{\mathrm{ND}} \min_{k=1,2,\cdots,NC}\left[\frac{C_{Dj,k}^{\lim}}{C_{Si,k}}\right]} \quad (i \neq j) \tag{7}$$

From Eqs. 4 and 7, it can be seen that both the CPD and CPS values are the functions of the contaminant concentrations. If there are a few demand streams (or source streams) with the same concentrations, they should be treated as one stream in the calculation of CPD and CPS.

In the following discussion, we will use an example to show that the CPD and CPS defined earlier are reliable. Table 2 lists the concentration potentials of the streams for the system shown in Table 1. Table 3 compares the order of the CPDs with that of the conventional limiting inlet concentrations of the example. From Table 3, it can be seen that the order of the CPDs of D_3, D_7, D_5, and D_6 agrees with the order of the conventional concentrations of D_3, D_7, D_5, and D_6. The same conclusion can be obtained from the comparison of the order of the CPDs and that of the conventional concentrations for the other demand streams, as shown in Table 3. That means, the order of the limiting inlet concentration potentials CPDs agrees with that of the conventional limiting inlet concentrations. Similarly, from Table 4, it can be seen that the order of the CPSs agrees with that of the conventional limiting concentrations of the source streams. From this example, it can be seen that the concentration potentials proposed are reliable.

Allocation of Source Streams to Demand Streams

When demands are satisfied by sources, the mass loads of the contaminants will play an important role. The mass load(s) of the RKC(s) might reach the limiting value(s), if the amount of the source is sufficient. However, the mass loads of the non-RKCs cannot reach their limiting values. Let us consider the example shown in Table 1. For D_3, the mass loads of contaminants *A, B,* and *C* (in kg/h) are 3, 4.5, and 1.5, respectively. For S_1, the mass loads of the contaminants are 3, 2.7, and 1.5, respectively. If D_3 is satisfied by S_1, $C_{D3,1}/C_{S1,1} = 0.4$, $C_{D3,2}/C_{S1,2} = 0.67$, and $C_{D3,3}/C_{S1,3} = 0.4$. The RKCs for this allocation are contaminants *A* and *C*. Both the mass loads of contaminants *A* and *C* in D_3 can be totally satisfied, as shown in Figure 1.

If D_3 is satisfied by S_2, $C_{D3,1}/C_{S2,1} = 0.8$, $C_{D3,2}/C_{S2,2} = 0.86$, and $C_{D3,3}/C_{S2,3} = 0.29$. The RKC for this allocation is contaminant *C*. Only contaminant *C* in demand D_3 could be totally satisfied, if the amount of S_2 would be sufficient. However, because the amount of S_2 is not sufficient, none of the contaminants can be totally satisfied, as shown in Figure 2a. The remaining mass loads of the contaminants after allocation of (S_2, D_3), as shown in Figure 2b, can be satisfied by another source.

When there are many source streams available, we should decide which source should be reused first. To reduce freshwater consumption, the source with the largest value of the maximum quasi-allocation amount, which can be calculated from Eq. 3, should be used first. If there are a few sources with the same maximum quasi-allocation amount for a demand, the source stream with the highest CPS value should be reused to reduce freshwater consumption of the downstream processes, where the CPS values of the sources should be calculated based on the unperformed processes. If the demand cannot be totally satisfied by one source, as shown in Figure 2, another source should be used. The remainder of the mass loads in the demand can be calculated by subtracting the mass loads in the source, which have been allocated, from the maximum mass loads of the demand. The remainder of the mass loads of the demand and the maximum flowrate of the process can be used to calculate the remaining concentrations of the contaminants. Similar proce-

Table 3. Comparison of the Order of the *CPDs* and That of the Conventional Concentrations for Example 1

Stream	CPD	CC (ppm)	Stream	CPD	CC (ppm)	Stream	CPD	CC (ppm)
D_3	1.48	40, 60, 20	D_4	1.54	30, 40, 70	D_8	2.45	90, 50, 34
D_7	1.66	100, 75, 20	D_6	9.00	200, 170, 150	D_5	4.52	110, 135, 60
D_5	4.52	110, 135, 60				D_6	9.00	200, 170, 150
D_6	9.00	200, 170, 150						

CC, conventional concentration.

Table 4. Comparison of the Order of the *CPSs* and That of the Conventional Concentrations for Example 1

Stream	CPS(S_i)	CC (ppm)	Stream	CPS(S_i)	CC (ppm)
S_2	0.22	50, 70, 70			
S_3	0.33	150, 80, 70	S_1	0.22	100, 90, 50
S_4	0.37	160, 100, 90	S_4	0.37	160, 100, 90
S_8	0.50	210, 170, 100	S_8	0.50	210, 170, 100
S_5	0.63	210, 200, 120	S_5	0.63	210, 200, 120
S_7	0.75	300, 290, 170	S_7	0.75	300, 290, 170
S_6	1.46	350, 400, 210	S_6	1.46	350, 400, 210

CC, conventional concentration.

dure as mentioned earlier can be used to choose the source for allocating to the remainder of the demand stream. The allocation procedure will continue till the concentration(s) of at least one contaminant reach the maximum.

When the real concentrations of the demand, which are often different from the limiting ones, are determined, the final outlet concentrations of the process can be calculated by adding the concentration increment caused by the mass loads of the contaminants removed in the process.

When only freshwater is used, it is possible to make the outlet concentrations of at least one contaminant reach the maximum value(s). The contaminant(s) whose concentration(s) reach the maximum value(s) first will determine the minimum freshwater amount $F_{\text{fresh}}^{\min}$, when only freshwater is used:

$$F_{\text{fresh}}^{\min} = \max_{k=1,2,\cdots,\text{NC}} \left[\frac{m_k^{\text{rem}}}{C_k^{\text{lim,out}}} \right] \quad (8)$$

where m_k^{rem} is the mass load of contaminant k removed in the process, and $C_k^{\text{lim,out}}$ is the limiting outlet concentration of contaminant k in the process.

We call the contaminant(s), which corresponds to $F_{\text{fresh}}^{\min}$, as the freshwater key contaminants (FKCs).

For a process of single contaminant, if the concentration of a source is higher than the limiting outlet concentration of the process, it is not necessary to reuse the source, because freshwater consumption cannot be reduced compared with the amount of freshwater $F_{\text{fresh}}^{\min}$ obtained by Eq. 8. For a process of multiple contaminants, when a source is allocated to the demand of the process, if the RKC and the FKC are the same contaminant, and if the concentration of the key contaminant of the source is higher than the corresponding limiting outlet concentration of the process, we will not reuse this source, because freshwater consumption cannot be reduced compared with the amount of freshwater $F_{\text{fresh}}^{\min}$ obtained by Eq. 8. In this situation, we will use freshwater solely instead.

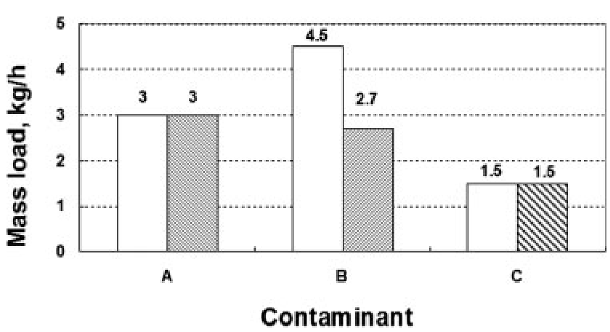

Figure 1. Demand D_3 is satisfied by S_1 for the example shown in Table 1, where the shadowed areas represent the mass loads of the sources and the nonshadowed areas represent the mass loads of the demands.

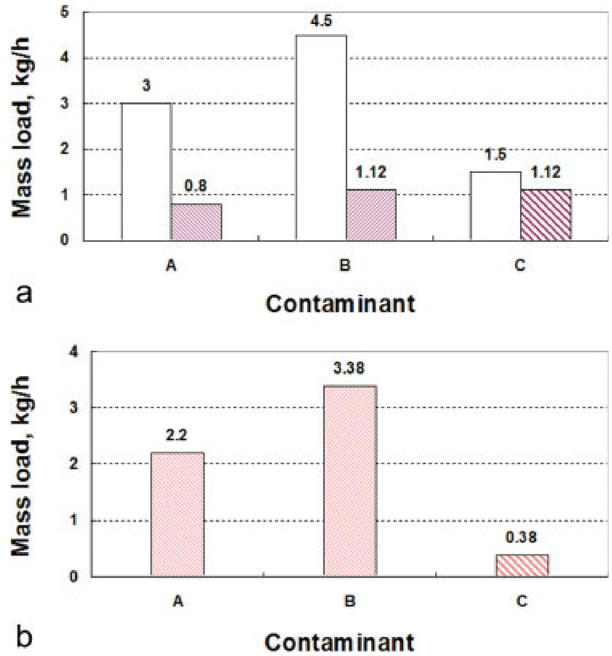

Figure 2. Demand D_3 is satisfied by S_2 for the example shown in Table 1.

(a) Demand D_3 cannot be totally satisfied by S_2. (b) The remainder mass loads after allocation of (S_2, D_3). [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Proposed Design Procedure

In this article, the inlet concentration potential will be taken as the main factor to decide the performing order of the processes. We will use the similar rules which were used for design of the water-using networks proposed by Liu et al.[22] The design procedure proposed in this article is as follows:

(1) Arrange the processes in ascending order of the limiting inlet concentration potentials;

(2) The processes with the lowest limiting inlet concentration potentials will be performed first, and they often use

Table 5. Final Concentrations of the Streams of Example 1

	C_{in} (ppm)			C_{out} (ppm)		
Process	*A*	*B*	*C*	*A*	*B*	*C*
1	0	0	0	100	90	50
2	0	0	0	50	70	70
3	40	36	20	150	56	70
4	28.6	40	40	158.6	100	60
5	110	48.1	57.8	210	113.1	117.8
6	154.8	65.9	72.7	350.0	365.1	150.7
7	42.9	16	20	242.9	231	170
8	84.3	46.3	34	204.3	166.3	100

Where the concentrations reach their maximum are shadowed in the Table.

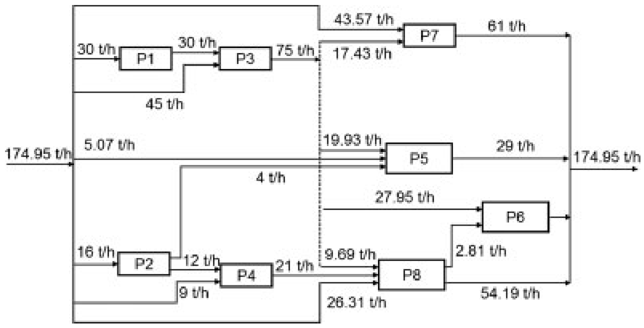

Figure 3. Design for Example 1.

freshwater;

(3) If a source stream is used up, it will not be considered in the following steps;

(4) The inlet concentration potentials of the processes to be performed will be calculated based on the current available sources, which are the outlet streams of the performed processes. The process with the lowest inlet concentration potential will be performed first. If there are a few processes with the same inlet concentration potentials, the process with the lowest outlet concentration potential will be performed first;

(5) Satisfy the demand stream by the current available sources and perform the process;

(6) Return to step (3), till all the processes are performed.

The allocation strategies in step 5 have been discussed in the section "Allocation of source streams to demand streams." We will summarize the procedure of allocations as follows:

(a) For the process being performed, find the source(s) with the largest quasi-allocation amount. If the quasi-allocation amounts of a few sources are the same, the source with the highest CPS value will be selected, and go to step (b);

(b) If the RKC and FKC are the same contaminant, and if the limiting outlet concentration of the key contaminant of the process is lower than that of the source, the source will not be reused. Instead, freshwater is used solely. Otherwise, allocate the sources to the demand, and go to step (c);

(c) If the demand is not totally satisfied, select the next source by using the similar procedure as mentioned in steps (a) and (b), till the demand is totally satisfied.

It should be pointed out that in the design procedure, if possible, the real concentrations and flow rates should be used in the calculations.

Table 6. Limiting Process Data for Example 2

Process	Contaminant	$C^{\max,\text{in}}$ (ppm)	$C^{\max,\text{out}}$ (ppm)	C^{rem} (g/h)
1	A	0	15	675
	B	0	400	18,000
	C	0	35	1575
2	A	20	120	3400
	B	300	12,500	414,800
	C	45	180	4590
3	A	120	220	801.2
	B	20	45	200.3
	C	200	125,000	1,000,000
4	A	0	22	418
	B	0	120	2280
	C	0	30	570
5	A	150	225	9750
	B	200	310	1300
	C	250	350	13,000
6	A	0	4.7	800
	B	0	1.2	200
	C	0	2000	340,000
7	A	100	270	4930
	B	20	3500	100,920
	C	50	250	5800

Table 7. Performing Order and Allocation of the Sources to the Demands of Example 2

Performing Order	Allocation	Amount (t/h)	Fresh water (t/h)
P_1			45
P_4			19
P_6			170
P_7	(S_4,D_7)	4.83	24.17
P_3	(S_4,D_3)	1.33	6.67
P_2	(S_4,D_2)	12.83	0
	(S_1,D_2)	21.15	
P_5	(S_1,D_5)	22.41	22.41 + 770

Case Studies

Example 1

This example is taken from Wang et al.,[12] with the data shown in Table 1. The values of CPDs and CPSs based on the limiting concentrations for the processes are listed in Table 2.

For this example, processes 1 and 2 will be performed first, because their limiting inlet concentration potentials are the lowest. Freshwater consumption amounts are 30 t/h and 16 t/h for processes 1 and 2, respectively.

Then, the CPD values of the demand streams of the unperformed processes can be calculated based on the current available sources, S_1 and S_2. It should be pointed out that the CPD values calculated based on the current available sources are different from those listed in Table 2, which are calculated based on the limiting concentrations. The CPD values of processes 3 and 7, which are calculated based on the current available sources, are the same (0.69), and they are the lowest. Therefore, either process 3 or process 7 should be performed now. The CPS value of the outlet stream of pro-

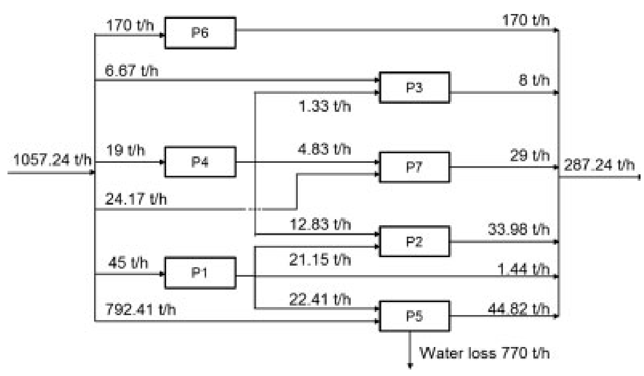

Figure 4. Design for Example 2.

Table 8. Final Concentrations of the Streams of Example 2

	C^{in} (ppm)			C^{out} (ppm)		
Process	*A*	*B*	*C*	*A*	*B*	*C*
1	0.0	0.0	0.0	15.0	400.0	35.0
2	17.6	294.3	33.1	117.7	12500.0	168.2
3	3.7	20.0	5.0	103.8	45.0	125000.0
4	0.0	0.0	0.0	22.0	120.0	30.0
5	7.5	200.0	17.5	225.0	229.0	307.5
6	0.0	0.0	0.0	4.7	1.2	2000.0
7	3.7	20.0	5.0	173.7	3500.0	205.0

Where the concentrations reach their maximum are shadowed in the Table.

cess 3 is lower than that of process 7. Therefore, process 3 should be performed first. For process 3, 30 t/h of S_1 can be used, because the maximum quasi-allocation amount of (S_1, D_3) is larger than that of (S_2, D_3). Freshwater consumption is 45 t/h.

Source 1 is used up now. Therefore, the CPD values of the unperformed processes should be calculated based on the current available sources, S_2 and S_3. From the CPD values, it can be seen that process 7 should be performed then. For process 7, the maximum quasi-allocation amount for (S_2, D_7) and that for (S_3, D_7) are the same. However, the CPS value of S_3 is higher. Therefore, S_3 is used first to reduce freshwater consumption of the downstream processes. The reuse amount of S_3 is 17.43 t/h and freshwater consumption is 43.57 t/h.

Process 4 is performed then. The reuse amount of S_2 is 12 t/h. Freshwater consumption is 9 t/h.

Based on the CPD values obtained from the current available sources, process 8 should be performed. Source 4 is used first because its quasi-allocation amount is the largest. The maximum quasi-allocation amount for (S_4, D_8) is 28.5 t/h, which is larger than the real amount of S_4. Then, 21 t/h of S_4 can be totally used for process 8. Then, 9.69 t/h of S_3 can be used. Freshwater consumption is 26.31 t/h.

The next performed process is process 5. For this process, the quasi-allocation amount of S_2 is the largest. The remainder of S_2, 4 t/h, is used first. Then, 19.93 t/h of S_3 can be used. Freshwater consumption is 5.07 t/h.

For process 6, the remainder of S_3 and 2.81 t/h of S_8 will be used. Freshwater is not required for this process.

The total freshwater consumption is 174.95 t/h, which is even lower than the minimum freshwater target value (177.1 t/h) reported by Wang et al.[12] The freshwater consumption of the design obtained in this work is significantly less than

Table 9. Limiting Process Data of Example 3

Process	Contaminant	F^{max} (t/h)	$C^{max,in}$ (ppm)	$C^{max,out}$ (ppm)
1	A	45	0	15
	B		0	400
	C		0	35
2	A	34	20	120
	B		300	12,500
	C		45	180
3	A	56	120	220
	B		20	45
	C		200	9500

Table 10. Performing Order and Allocation of the Sources to the Demands of Example 3

Performing Order	Allocation	Amount (t/h)	Fresh water (t/h)
P_1			45
P_3	(S_1, D_3)	2.8	53.2
P_2	(S_1, D_2)	25.5	8.5

198.4 t/h, which is obtained by Wang et al.[12] by using single internal water main approach. The final concentrations are shown in Table 5, in which the concentrations reach their maximum are shadowed. From the Table, it can be seen that for all the processes, the outlet concentrations of at least one contaminant reach the maximum, and the inlet concentrations of at least one contaminant reach the maximum, except process 6. The design is shown in Figure 3. From Figure 3, it can be seen that the interconnection number for the design of this work is 20, which is the same as that of the design of Wang et al.[12]

Example 2

This example is taken from Alva-Argáez et al.[14] with the data shown in Table 6. A fixed water loss of 770 t/h is assumed for the evaporative cooling system (process 5); the remaining flow is available for reuse and treatment.[14] The performing order and allocations of the sources to the demands are listed in Table 7. The design obtained is shown in Figure 4. The total freshwater consumption is 1057.24 t/h, which is 0.4% higher than the minimum freshwater consumption 1053.4 t/h reported by Alva-Argáez et al.,[14] who used a mixed-integer nonlinear programming approach to solve the problem. The interconnection number for the design of this work is 17 and that for the design of Alva-Argáez et al.[14] is 20. The final concentrations of the streams are shown in Table 8.

Example 3

The limiting data for Example 3 from Doyle and Smith[4] are shown in Table 9. The performing order and allocations of the sources to the demands are listed in Table 10. The design of this example is shown in Figure 5, which has the same structure as that shown in Figure 6b of Doyle and Smith.[4] The total freshwater consumption is 106.70 t/h, which is slightly larger than 105.65 t/h, the result of Doyle and Smith.[4] The final concentrations of the processes are listed in Table 11.

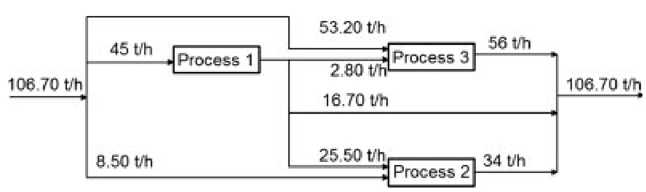

Figure 5. Design of Example 3.

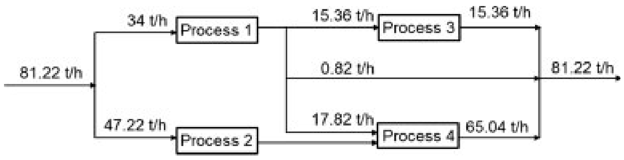

Figure 6. Design for Example 4.

Table 11. Final Concentrations of the Streams of Example 3

	C^{in} (ppm)			C^{out} (ppm)		
Process	*A*	*B*	*C*	*A*	*B*	*C*
1	0	0	0	15	400	35
2	11.3	300	26.3	111.3	12,500	161.3
3	0.8	20	1.8	100.8	45	9301.8

Where the concentrations reach their maximum are shadowed in the Table.

Example 4

The limiting data of Example 4 from Doyle and Smith[4] are listed in Table 12. The performing order and allocations of the sources to the demands are listed in Table 13. The total freshwater consumption is 81.22 t/h, which is the same as that of Doyle and Smith[4] who used a nonlinear programming method. The design is shown in Figure 6. From Table 13, process 2 should be performed after process 1. It should be pointed out that for process 2, the RKC for (S_1, D_2) and the FKC are the same: contaminant *B*. The limiting outlet concentrations of process 2, in ppm, are 300, **270**, and 740. The concentrations of S_1 are 160, **450**, and 30. The concentration of the key contaminant in S_1 (450 ppm) is even higher than that in the limiting outlet concentration of process 2 (270 ppm). Therefore, process 2 will use freshwater solely, and freshwater consumption is 47.22 t/h. The final concentrations of the processes are shown in Table 14.

Table 12. Limiting Process Data of Example 4

Process	Contaminant	F^{max} (t/h)	$C^{max,in}$ (ppm)	$C^{max,out}$ (ppm)
1	A	34	0	160
	B		0	450
	C		0	30
2	A	75	200	300
	B		100	270
	C		500	740
3	A	20	600	1240
	B		850	1400
	C		390	1580
4	A	80	300	800
	B		460	930
	C		400	900

Table 13. Performing Order and Allocation of the Sources to the Demands of Example 4

Performing Order	Allocation	Amount (t/h)	Fresh water (t/h)
P_1			34
P_2			47.22
P_4	(S_2, D_4)	47.22	0
	(S_1, D_4)	17.82	
P_3	(S_1, D_3)	15.36	0

Table 14. Final Concentrations of the Processes of Example 4

	C^{in} (ppm)			C^{out} (ppm)		
Process	*A*	*B*	*C*	*A*	*B*	*C*
1	0	0	0	160	450	30
2	0	0	0	158.8	270	381.2
3	160	450	30	993.6	1166.4	1580.0
4	159.1	319.4	284.8	774.2	897.4	900.0

Where the concentrations reach their maximum are shadowed in the Table.

Discussion and Conclusions

A heuristic procedure is proposed in this article to design the fixed-mass-load water-using networks with multiple contaminants. New methodology concepts, the concentration potentials of the demand (inlet) streams, and those of the source (outlet) streams, are introduced. The concentration potential of a demand reflects the overall possibility of the demand reusing the source streams, and the concentration potential of a source reflects the overall possibility of the source is reused by the demands. The order of the concentration potentials agrees with that of conventional concentrations. In the proposed design procedure, the performing order is determined according to the order of the inlet concentration potentials. The process with the lowest inlet concentration potential(s) will be performed first.

A few case studies are investigated. The results show that the method proposed can provide excellent designs for the water-using networks with multiple contaminants. The freshwater consumptions of the designs obtained in this work are very close to (even lower than) the target values reported in the literature. One of the most important advantages of the method proposed is that it can obtain a very good design in a noniterative way. The numbers of interconnections of the designs obtained in this work are not large compared with the designs obtained in the literature. That means the structure of the design obtained in this work is not complex.

If the design obtained by the method proposed is taken as the initial point for an optimization procedure, the optimization efficiency might be increased. The method is also useful as a shortcut model to evaluate the targets of the minimum freshwater consumption of the water-using networks with multiple contaminants.

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Notation

C = concentration
$C_{Dj,RKC}$ = concentration of the reuse key contaminant (RKC) in demand D_j

$C^{\lim}_{Dj,k}$ = limiting concentration of contaminant k in demand D_j
CPD(D_j) = concentration potential of demand D_j when only considering reuse, as defined by Eq. 4
CPS(S_i) = concentration potential of source S_i when only considering reuse, as defined by Eq. 7
$C_{Si,\mathrm{RKC}}$ = concentration of the reuse key contaminant (RKC) in source S_i
D_j = demand stream j
$F^{\min}_{\mathrm{fresh}}$ = minimum flowrate of the process when only freshwater is used
NC = number of the contaminants
ND = number of the demands
NS = number of the sources
RKC = reuse key contaminant
$R_{i,j}$ = maximum quasi-allocation amount from source S_i to 1 ton of demand D_j, as defined by Eq. 3
S_i = source stream i
(S_i, D_j) = allocation of source stream S_i to demand stream D_j

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