R&D NOTES

A Simple Method for Design of Water-Using Networks with Multiple Contaminants Involving Regeneration Reuse

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Introduction

Water-using system optimization is a very important research in chemical engineering field. Many methods have been proposed to deal with wastewater minimization for single contaminant systems.[1–9] The design and targeting of the water networks with multiple contaminants have also been investigated.[1,4,10–22] When regeneration is introduced in a water network, freshwater consumption will be reduced further compared with the networks involving reuse only.[8,12,13]

Kuo and Smith[12,13] proposed a systematic method for design of the water networks with multiple contaminants involving regeneration. The method includes three stages: pinch identification, operation grouping, and operation migration. The pinch point and the target of the network involving reuse only are determined first. Then, the operations are divided into two groups according to the freshwater pinch point for the system involving reuse only. According to Kuo and Smith[13]: initially, operations entirely below the freshwater pinch belong with Group I and are used for freshwater targeting; operations across or above the freshwater pinch belong to Group II and are used for regeneration targeting. The processes in Group I will be fed by freshwater, and the processes in Group II will be fed by the regenerated water. The two groups are designed separately. Operation migrations between the two groups are then carried out based on the two mechanisms and seven criteria proposed by Kuo and Smith[13] to find the final design for the water networks with regeneration. From the above discussion, it can be seen that the design procedure of Kuo and Smith[13] is complex.

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In this article, a new method will be proposed to design the water-using systems with one regeneration stream. By analysis, a new insight is obtained that the difference between the network involving regeneration reuse and that involving reuse only is that there is an additional source, the regenerated stream, in the former network. Adding the regenerated source in the sources of the network involving reuse only, the design of the networks involving regeneration reuse can be carried out by using the design procedure proposed for the systems involving reuse only, such as the methods proposed by Liu et al.[4,18] However, the concentration(s) and flowrate of the regenerated source are not known before detailed design of the network involving regeneration reuse. To determine the concentration(s) and flowrate of the regenerated source, the whole network is divided into two parts: the subnetwork before regeneration and that after regeneration. By designing of the subnetwork before regeneration, the flowrate and concentration(s) of the regenerated source can be obtained. The design procedure proposed is simpler than the method of Kuo and Smith.[12,13] The results obtained in this work are comparable with that obtained by Kuo and Smith.[12,13]

The new method

For the water-using networks with multiple contaminants involving reuse only, Liu et al.[4] proposed heuristic rules: (1) perform the processes starting with the lowest limiting inlet concentrations of contaminants; (2) for the processes with the same limiting inlet concentrations, water should be allocated first to the process with the lowest limiting outlet concentrations. In the work of Liu et al.,[18] new methodology concepts, the concentration potentials of the demand (inlet) streams (CPDs) and the concentration potentials of the source (outlet) streams (CPSs) are introduced. The process

Table 1. Limiting Data for Example 1

Process	m (kg/h)	C_{in} (ppm)	C_{out} (ppm)	F_{max} (t/h)
1	8	0	200	40
2	5	100	200	50
3	9	100	400	30
4	6	300	400	60
5	8	400	600	40

sequence is determined by the order of the concentration potentials of the demands.[18]

Let us discuss briefly the concepts of the CPD and CPS. The readers are referred to the work of Liu et al.[18] for more information. The CPD value of a demand is a measurement of the overall possibility of the demand to reuse the source streams, as shown in Eq. 1:

$$\mathrm{CPD}(D_j) = \sum_{i=1}^{N_S} \min_{k=1,2,\ldots,N_C} \left[\frac{C_{D_j,k}^{\lim}}{C_{S_i,k}} \right] \quad (i \neq j) \tag{1}$$

where $i \neq j$ because recycling is not considered in this work, $C_{D_j,k}^{\lim}$ is the limiting concentration of contaminant k in demand D_j, $C_{S_i,k}$ is the concentration of contaminant k in source S_i, N_C is the number of the contaminants, and N_S is the number of the source streams.

The CPS value of a source stream is a measurement of the overall possibility of the source to be reused by the demand streams, as shown in Eq. 2:

$$CPS(S_i) = \frac{1}{\sum_{j=1}^{N_D} \min_{k=1,2,\ldots,N_C} \left[\frac{C_{D_j,k}^{\lim}}{C_{S_i,k}} \right]} \quad (i \neq j) \tag{2}$$

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

The results of a few case studies show that the method of Liu et al.[18] can give very good designs for the water-using networks of multiple contaminants involving reuse. In this work, the methods of Liu et al.[4,18] will be extended to the water-using networks involving regeneration reuse.

According to Kuo and Smith,[13] the following simple measure (removal ratio, RR) can be used to define the performance of a regeneration process:

$$\mathrm{RR} = \frac{f_{in}C_{in} - f_{out}C_{out}}{f_{in}C_{in}} \tag{3}$$

We call the contaminants removed in a regeneration process as the determining-contaminants (DCs) for the regeneration process. For convenience, we call the design involving reuse only as the reuse-design (RD), and that involving regeneration reuse as the regeneration-reuse-design (RRD). Generally speaking, the RRD is significantly different from the RD. Let us discuss the difference between the RD and RRD by analysis of Example 1.

Example 1. This is a single contaminant system with the data shown in Table 1, taken from Kuo and Smith.[13] Freshwater consumption for the RD (Figure 1a) and that for the RRD (Figure 1b) are 80 and 44 t/h, respectively.[13] From Figures 1a, b, it can be seen that the skeleton of the RD and that of the RRD are almost totally different, even though the design specifications of the two designs are the same. What causes the difference? Compared to the RD, it can be seen that there is an additional source stream, the regenerated stream (S_{reg}), in the RRD. It is the regenerated stream S_{reg} that causes the difference between the RRD and the RD: the freshwater targets are not the same; the pinch points might not be the same; the wastewater targets will not be the same. Because the design specifications of the RD and those of the RRD are the same, if we can obtain the flowrate and concentration(s) of the S_{reg}, and include the S_{reg} in the sources of the RD, we can obtain the RRD by using the design method proposed for the RD. Now, the question is how to determine the concentration(s) and flowrate of the S_{reg} before we obtain the RRD.

Generally speaking, as a rule of thumb (Feng et al.[8]), the concentration of the S_{reg} (C_{reg}) might be assumed to be the lowest concentrations of the demand C_{DL} (except 0) of all the processes. In this work, we assume:

$$0 < C_{reg} \leq C_{DL} \tag{4}$$

Although the concentration of the S_{reg} is not known before designing of the RRD, the limiting regenerated concentration of a process, $C_{reg}^{\lim}$, can be estimated from the RR value defined in Eq. 3 and the limiting outlet concentration of the process as follows:

$$C_{reg}^{\lim} = C_{out}^{\lim} \times (1 - \mathrm{RR}) \tag{5}$$

To reduce the regeneration cost, if the $C_{reg}^{\lim}$ meets the conditions of formula 4, the flowrate of the regenerated stream should be as small as possible, because regeneration cost can be assumed as a function of the RR value and the total flow of wastewater requiring treatment.[16] If the $C_{reg}^{\lim}$ of a stream

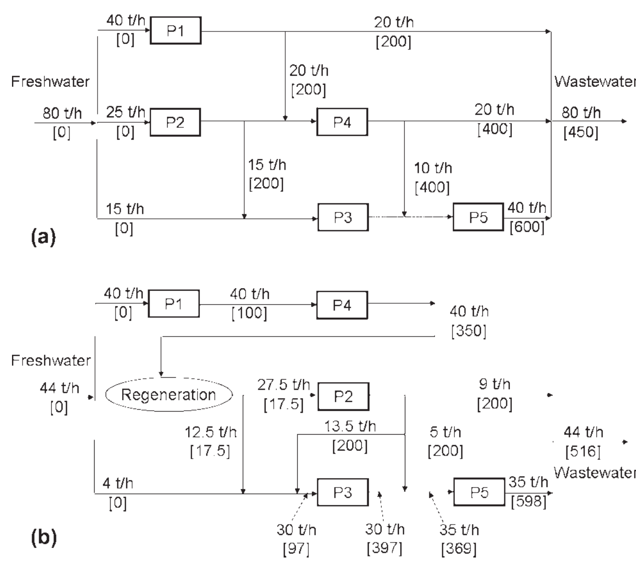

Figure 1. Design for Example 1 obtained by Kuo and Smith,[13] where the numbers in the brackets are the concentrations in ppm. Design for (a) maximum reuse; (b) regeneration reuse.

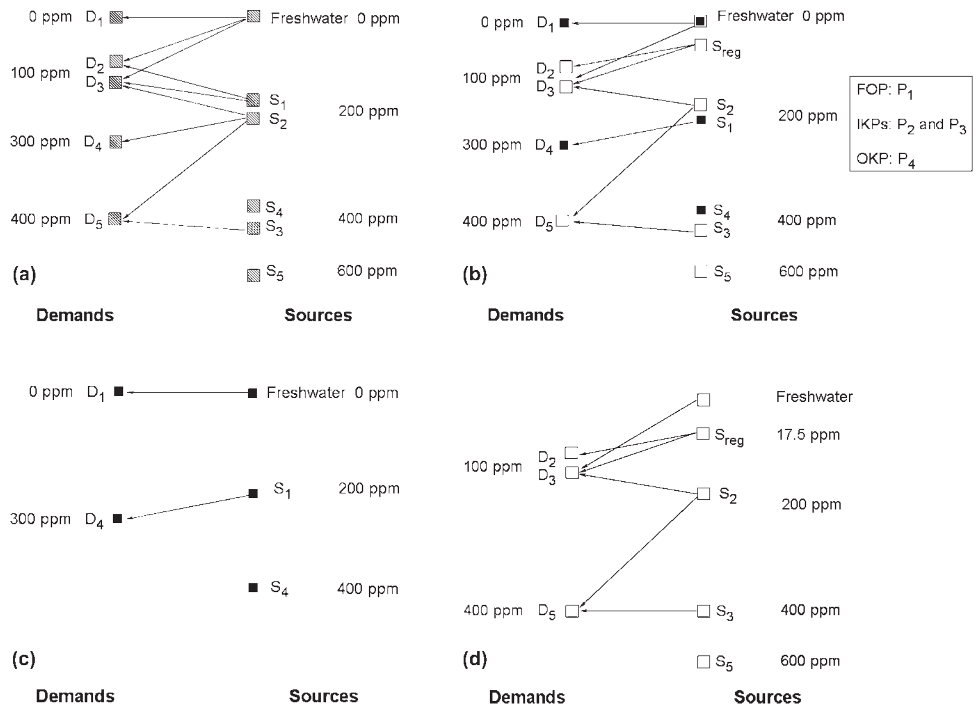

Figure 2. Allocations from the sources to the demands in a few systems.

(a) Network of a RD (different from that shown in Figure 1a); (b) network of a RRD; (c) subnetwork before regeneration; (d) subnetwork after regeneration. (b–d) The solid squares illustrate the stream not connected to the S_{reg}, and the hollow squares illustrate the stream connected to the S_{reg}.

is very high, the stream should not be regenerated for reuse. Based on the above analysis, the regeneration stream can be determined initially.

For this example, from the data in Table 1 and the RR value (95%), if all the outlet streams are regenerated, the limiting regenerated concentrations of the streams $(C_{reg}^{lim})s$ can be calculated from Eq. 5, and their values are: 10, 10, 20, 20, and 30 ppm, respectively. The lowest concentration of the demand except 0 is 100 ppm: $C_{DL} = 100$ ppm. All the $(C_{reg}^{lim})s$ meet the conditions of formula 4, if the source streams are regenerated. It can be seen that S_4 and/or S_5 can be regenerated for reuse. However, the source streams S_1, S_2, and S_3 will not be regenerated because that will incur recycling, if they are regenerated. There might be three options to regenerate S_4 and/or S_5: to regenerate S_4 only, to regenerate S_5 only, and to regenerate both S_4 and S_5.

To compare the design with reuse only and the design involving regeneration reuse, let us consider the design with reuse briefly. Based on the design procedure of Liu et al.,[4] for a system of single contaminant, when only reuse is considered, the source streams and the demand streams will be arranged in the ascending concentration order first, respectively. The processes with the lowest inlet concentrations should use freshwater solely (such as process 1 in this example). We call the processes which need freshwater only as the Freshwater Only Processes (FOPs). The other demand streams will then be satisfied by the source streams in turn. For example, Figure 2a shows the allocations from the sources to the demands of a RD for Example 1. Please note that the design shown in Figure 2a is different from that of Figure 1a.

Let us analyze how a regenerated source affects the design by using Figure 2b, in which S_4 is regenerated. The detailed design of this system will be discussed in the next section. In Figure 2b, the process streams connected to the S_{reg} are illustrated by hollow squares, and those not connected to the S_{reg} by solid squares. For a RRD, the demand streams of the FOPs will be satisfied by freshwater solely as well. However, the allocations from the sources to the demands, whose concentrations are higher than the C_{reg}, will be different from those in the RD, because of the introduction of the S_{reg}. For example, the demands whose concentrations are just higher than the C_{reg}, D_2 and D_3 in Figure 2b, will reuse the S_{reg}. On the other hand, in the RD shown in Figure 2a, D_2 and D_3 reuse S_1. We call the processes, which reuse the S_{reg}, as the inlet key processes (IKPs), because their inlet concentrations should be low.

The demand D_4 will reuse S_1. The outlet stream of process 4, S_4, will be regenerated for reuse. We call the process whose outlet stream will be regenerated as the outlet key process (OKP), because its outlet concentration is important for the regeneration process. The demand D_5 can be satisfied by S_2 and S_3. It should be pointed out that process 5 is neither an IKP nor an OKP, in this case.

From the above discussion, it can be seen that the whole network of the RRD in Figure 2b can be divided into two subnetworks: the one after regeneration which includes the processes and streams connected to the S_{reg}, and the one before regeneration which includes the processes and streams

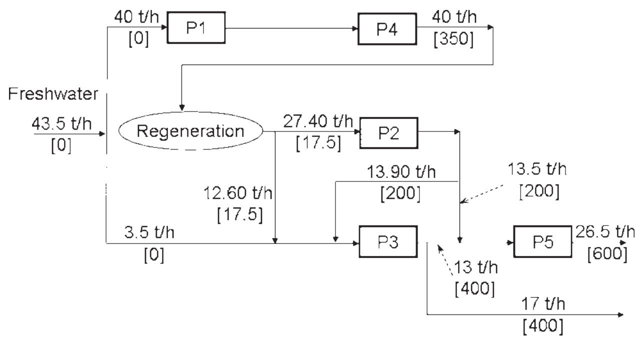

Figure 3. Final design for Example 1 obtained in this work.

not connected to the S_{reg}. Figure 2c shows the subnetwork before regeneration, and Figure 2d shows the subnetwork after regeneration. By designing of the subnetwork before regeneration, the concentration(s) and flowrate of the stream to be regenerated can be obtained. From the concentration(s) of the stream to be regenerated and the RR value defined by Eq. 3, the final concentration(s) of the S_{reg} can be obtained. Then, the detailed design of the RRD can be carried out by using the same design procedure proposed for the RD.

We summarize the design procedure as follows:

1. Determine the DCs according to the regeneration process;
2. Identify the FOPs first;
3. Determine the S_{reg} which should meet formula 4 and not incur recycling. Include the S_{reg} in the source list according to its concentration. Then, determine the OKPs and the IKPs;
4. Develop and design the subnetwork before regeneration to determine the flowrate and concentration(s) of the S_{reg};
5. Include the data of the S_{reg} in the data of the RD sources. Then, the RRD can be obtained by using the design procedure proposed for the RD, such as the methods of Liu et al. [4,18]

Examples

Let us revisit "Example 1". We will discuss the system in which S_4 is regenerated. From the subnetwork before regeneration as shown in Figure 2c, the S_{reg} can be obtained as follows: P_1 uses 40 t/h of freshwater. For P_4, S_1 is reused. The concentration of S_4 is 350 ppm. The regenerated concentration is: $350 \times (1–0.95) = 17.5$ ppm, and the flowrate of the S_{reg} is 40 t/h.

Adding the S_{reg} in the sources in Table 1, we can obtain the whole data of the RRD. By using the targeting procedure of Liu et al.,[9] it can be obtained that the minimum freshwater requirement target is 43.5 t/h. Now, let us consider how to design a RRD which meets this target. Process 1 uses 40 t/h of freshwater. Demand D_2 can be satisfied by the S_{reg}. Let x be the flowrate of the S_{reg} required by D_2. By mass balance of the contaminant, we have: $17.5\,x + 5000 = 200\,x$, where 5000 g/h is the mass load of contaminant in P_2, and 200 ppm is the outlet concentration of P_2. Solving, we obtain: $x = 27.40$ t/h. Similarly, the flowrates and concentrations of the other streams can be obtained. The remainder 12.60 t/h of the S_{reg}, 13.90 t/h of S_2 and 3.5 t/h of freshwater can be used by D_3. Demand D_4 will reuse S_1. Then, D_5 will be satisfied by the remainder of S_2 with amount of 13.5 t/h and 13 t/h of S_3. The final design is shown in Figure 3. The freshwater requirement for the design obtained meets the target obtained above, 43.5 t/h, which is smaller than the freshwater requirement (44 t/h) of the design obtained by Kuo and Smith.[13] In the work of Kuo and Smith,[13] five operation migration steps were required to obtain the final design as shown in Figure 1b. It can be seen that the design procedure proposed in this work is simpler than that of Kuo and Smith.[13] In addition, the design when S_5 is regenerated, and that when both S_4 and S_5 are regenerated, can be obtained by using the method proposed in this work similarly.

Example 2

In this article, the case study example of Kuo and Smith[13] will be investigated, with the data shown in Table 2. The RR values for the regeneration process are: (0, 99.9%, 0) for contaminants A, B, and C, respectively. The determining-contaminant for the regeneration is contaminant B. Processes P_1 and P_4 are the FOPs, because they should use freshwater.

The $(C_{\text{reg}}^{\text{lim}})s$ of P_2, P_3 and P_5 are, in ppm: (120, 12.5, 180), (220, 0.045, 9500), and (150, 8, 120), respectively. From the data, it can be seen that both $S_{\text{reg},2}^{\text{lim}}$ and $S_{\text{reg},5}^{\text{lim}}$ can be reused for P_3. Source S_3 will not be regenerated for reuse, because the limiting regenerated concentration of contaminant C is too high. From the above analysis, the OKPs will be P_2 and P_5, and the IKP is P_3. The subnetwork before regeneration includes the FOPs (P_1 and P_4), and the OKPs (P_2 and P_5).

In this work, the design procedure proposed by Liu et al.[18] will be used to design both the subnetwork before regeneration and the RRD. According to Liu et al.,[18] the demand of the process with the lowest CPD value will be satisfied first. When a demand is satisfied, the source with the largest quasi-allocation amount, as defined in Eq. 6, will be reused first.[18]

$$R_{i,j} = \min_{k=1,2,\ldots,N_C} \left(\frac{C_{D_j,k}^{\text{lim}}}{C_{S_i,k}} \right) \tag{6}$$

Now, let us design the subnetwork before regeneration. Processes 1 and 4 use freshwater, 50 and 8 t/h, respectively. From the current available source streams, S_1 and S_4, the CPD values of D_2 and D_5 can be calculated. For example:

Table 2. Limiting Data for Example 2

Process	Contaminant	C_{in} (ppm)	C_{out} (ppm)	$F_{\max}$ (t/h)
1	A	0	15	50
	B	0	400	
	C	0	35	
2	A	20	120	34
	B	300	12500	
	C	45	180	
3	A	120	220	56
	B	20	45	
	C	200	9500	
4	A	0	20	8
	B	0	60	
	C	0	20	
5	A	50	150	8
	B	400	8000	
	C	60	120	

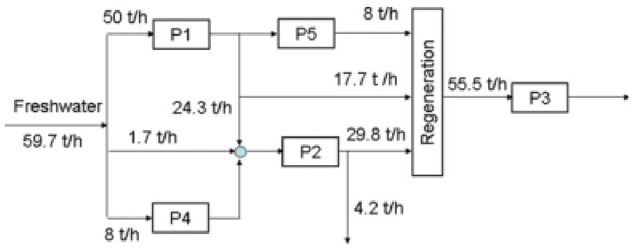

Figure 4. Final design for Example 2 obtained in this work.

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

$$\mathrm{CPD}(D_2) = \min\left(\frac{C^{\lim}_{D2,1}}{C_{S1,1}}, \frac{C^{\lim}_{D2,2}}{C_{S1,2}}, \frac{C^{\lim}_{D2,3}}{C_{S1,3}}\right) + \min\left(\frac{C^{\lim}_{D2,1}}{C_{S4,1}}, \frac{C^{\lim}_{D2,2}}{C_{S4,2}}, \frac{C^{\lim}_{D2,3}}{C_{S4,3}}\right) = \min\left(\frac{20}{15}, \frac{300}{400}, \frac{45}{35}\right) + \min\left(\frac{20}{20}, \frac{300}{60}, \frac{45}{20}\right) = 0.75 + 1 = 1.75$$

Similarly, we can obtain that $\mathrm{CPD}(D_5) = 3.5$. According to the design procedure of Liu et al.,[18] P_2 should be performed before P_5, because the CPD value of P_2 is smaller than that of P_5. For P_2, S_4 will be totally reused, and then 24.3 t/h of S_1 will be used. Freshwater consumption is 1.7 t/h.

For P_5, 8 t/h of S_1 can be reused. The sources S_2, S_5 and the remainder of S_1 can be mixed and regenerated. The flowrate of the mixed stream is 59.7 t/h. The concentrations of the mixed stream are, in ppm, (85.6, 8309, 116.9). The mixed stream is regenerated, and the concentrations of the regenerated source will be (85.6, 8.31, 116.9).

Adding the regenerated source in the sources of Table 2, we obtain the whole data for the RRD. The design of the RRD can start. Processes 1 and 4 use freshwater, 50 and 8 t/h, respectively. Based on the current available sources (S_1, S_4, and S_{reg}), the CPD values for D_2, D_3, and D_5 are 1.98, 1.79, and 4.01, respectively. The CPD values for D_2 and D_5 are not the same as those obtained above, because the S_{reg} is included in the sources now.

From the CPD values, D_3 should be satisfied before D_2 and D_5. For D_3, 55.5 t/h of the S_{reg}, the source with the largest quasi-allocation amount, can be reused. The design of P_2 and P_5 is the same as that of the subnetwork before regeneration. The flowrate of S_{reg} required by P_3 is 55.5 t/h, which is smaller than the flowrate of the S_{reg}, 59.7 t/h. Then, this design can be changed slightly, and the final design is shown in Figure 4. The final concentrations of the streams are shown in Table 3. The freshwater consumption of the design is 59.7 t/h, which is the same as that obtained by Kuo and Smith.[13] However, the design obtained in this work is slightly different from that obtained by Kuo and Smith.[13] In the work of Kuo and Smith,[13] after initial design and grouping, three operation migration steps were required to obtain the final design involving regeneration reuse. From the above discussion, it can be seen that the design procedure proposed in this paper is simpler than that of Kuo and Smith.[13]

Table 3. Final Concentrations and Flowrates of the Process Streams for Example 2

Process	Contaminant	C_{in} (ppm)	C_{out} (ppm)	F (t/h)
1	A	0	15	50
	B	0	400	
	C	0	35	
2	A	15	115	34
	B	300	12500	
	C	30	165	
3	A	83	184	55.5
	B	8	33	
	C	113	9500	
4	A	0	20	8
	B	0	60	
	C	0	20	
5	A	15	115	8
	B	400	8000	
	C	35	95	

The maximum concentrations are shadowed in the table.

Discussion and Conclusions

In this paper, a new design procedure is proposed for the water-using systems involving regeneration reuse, based on the new insight gained that the regenerated stream can be treated as an additional source stream to the water-using network involving reuse only. Then, the complex task of designing the network involving regeneration reuse can be converted to a simple task of determining the flowrate and concentration(s) of the regenerated stream. This simplifies the design of the network involving regeneration reuse, compared with the literature methods, such as the work of Kuo and Smith.[12,13] The results obtained in this work are comparable with that obtained in the literature. In this work, the concentration(s) of the regenerated source are assumed to be lower or equal to the lowest concentrations of the demand except zero. However, when the concentration(s) of the regenerated source being out of the range assumed, the method can still be used.

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Notation

$C^{\lim}_{D_j,k}$ = limiting concentration of contaminant k in demand D_j, ppm
C_{DL} = the lowest concentration of the demand except 0 ppm, ppm
CPD = concentration potential of the demand (inlet) stream as shown in Eq. 1
CPS = concentration potential of the source (outlet) stream as shown in Eq. 2
C_{reg} = concentration of the regenerated stream, ppm
$C^{\lim}_{\mathrm{reg}}$ = limiting concentration of the regenerated stream, ppm
$C_{S_i,k}$ = concentration of contaminant k in source S_i, ppm
D_j = demand j
DC = determining-contaminant for the regeneration
FOP = freshwater only process
IKP = inlet key process

N_C = number of the contaminants
N_D = number of demand streams
N_S = number of the source streams
OKP = outlet key process
RD = reuse-design
RR = removal ratio as shown in Equation 3
RRD = regeneration-reuse-design
S_i = source i
S_{reg} = regenerated stream

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