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# An Iterative and Subnetwork-Dividing Method to Design Multicontaminants Water-using Networks with Multiple Regeneration Units

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In the field of chemical engineering, when the regeneration recycling process is introduced into the waterusing networks (WUNs), several parameters that affect the cost of WUN can be reduced: the consumptions of freshwater and the regenerated water, and the wastewater discharge. However, it is often difficult to design the WUNs involving regeneration recycling and multiple regeneration units. This article introduced a subnetwork-dividing method to design WUNs involving regeneration recycling and multiple regenerated water. This method minimizes the consumption of freshwater and reduces the consumption of regenerated water. The main steps of the proposed method include: dividing of the whole network as pre-regeneration subnetwork and regeneration subnetwork, and design of subnetworks to obtain the final results. The results of a literature example: the consumption of freshwater is 58 t/h and the consumption of regenerated water is 179.143 t/h, it can be seen that method proposed in this paper is simple and effective. The design results obtained by this work are comparable to that obtained in the literatures.

# 1. Introduction

In the chemical engineering field, the design of WUNs is a highly valued research. Some researchers have used water pinch methods to study the design of WUNs. Wang and Smith (1994) proposed a graphical method, which can be used to design WUNs containing wastewater reuse and regeneration reuse. Mohammadnejad and Bidhendi (2011) proposed an appropriate method in which three contaminants were considered. Through the feasibility analysis of the regeneration reuse and recycling, they minimized the wastewater in the WUN.

Some researchers used mathematical programming methods to study the design of WUNs. Huang et al. (1999) proposed a mathematical programming model that can be used to design the optimal water-using and treatment network for any chemical plant. Their proposed method can make freshwater consumption and/or wastewater minimized. Faria et al. (2009) have developed a non-linear program (NLP) model that can be used to minimize the freshwater consumption and/or operating costs for networks with and without regeneration. Different types of water-using networks have also been designed: regeneration reuse WUNs and regeneration recycling water-using networks.

For the regeneration-reuse network, Bai et al. (2007) optimized the WUN with single-contaminant. The optimization results show that factors such as freshwater consumption and regenerated water flowrate can reach the minimum value. Hu et al. (2011) explored a method to determine the interim concentrations for concentration decomposition, and amount of freshwater and wastewater were reduced.

WUNs with the regeneration recycling process has been paid more attention. Kuo and Smith (1998) introduced a method to determine regeneration opportunities. The amount of water and wastewater produced can be reduced through proper use of regeneration reuse and regeneration recycling. Gomes et al. (2007) proposed the water source diagram procedure (WSD), a heuristic algorithm procedure. This procedure can design networks for different situations such as water re-use and regeneration recycling to minimize industrial water use. Souza et al. (2009) studied the implementation of the water source diagram (WSD) in petroleum refineries to minimize industrial water use. Li and Guan (2016) developed a stepwise optimization design

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approach for WUNs. The method can provide a WUN with regeneration reuse, this WUN has the minimum consumption of freshwater. Mabitla and Majozi (2019) have improved the graphics technology composite table algorithm (CTA) to determine the optimal removal rate of the regeneration unit and to minimize the consumption of freshwater. Wang et al. (2016) provided a wastewater treatment model for the water network. Li and Majozi (2017) proposed water networks with flexible framework, reduced freshwater consumption and wastewater discharge. According to the literatures, the regeneration units model of this work is fixed removal ratio type (Faria and Bagajewicz, 2011), and the fixed removal ratio is defined as shown in the Eq (1):

$$RR = \frac{f_{in}C_{in} - f_{out}C_{out}}{f_{in}C_{in}}$$
(1)

Liu et al. (2009a) introduced a method for design of water-using networks with one regeneration unit. However, based on Liu et al. (2009a), in this work, in this work, an iterative and subnetwork-dividing method will be introduced to design WUNs with multiple regeneration units and multiple contaminants, and there are discharge limits for wastewater from water-using networks. The division of subnetworks is occasionally not very accurate. The objective of this work is to reduce the flowrate of regenerated water. A new method of iterative and subnetwork-dividing is used, and the flowrate of regenerated water is reduced by 25%.

## 2. Concept of CPD and CPS

Liu et al. (2009b) proposed the concept of the concentration potential of demand streams (CPDs) and concentration potential of source streams (CPSs). CPD is defined as Eq (2):

$$CPD(D_{j}) = \sum_{i=1}^{NS} \min_{k=1,2,\cdots,NC} \left( \frac{C_{D_{j,k}}}{C_{S_{i,k}}} \right)$$
(2)

CPS is defined as Eq (3):

$$CPS(S_i) = \frac{1}{\sum_{i=1}^{ND} \min_{k=1,2,\cdots,NC} \left(\frac{C_{D_{i,k}}}{C_{S_{i,k}}}\right)}$$
(3)

Limiting quasi-allocation ratio value is defined as Eq (4):

$$\mathsf{R}_{i,j} = \min_{k=1,2,L,\mathsf{NC}} \left( \frac{\mathsf{C}_{\mathsf{D}_{j,k}}}{\mathsf{C}_{\mathsf{S}_{i,k}}} \right) \tag{4}$$

#### 3. Methodology

As mentioned above, the subnetwork-dividing method introduced in this paper include two main steps: determining the pre-regeneration subnetwork and regeneration subnetwork, and design of subnetworks to obtain the results.

#### 3.1 Division of subnetworks

This step is critical, the appropriate dividing of subnetwork can reduce the regenerated streams flowrate.

First, the water-using processes are defined as three types: FOP (Fresh water only process), the processes of using solely fresh water, IBP (Inlet concentration Below average Process) and OEP (Outlet concentration Exceed average Process). The limiting data is used to calculate CPDs and CPSs for all water-using processes. The average CPD value and the average CPS value can be calculated. The processes with CPD value equal to 0 are FOPs. The processes with CPD value lower than the average CPD value of all processes are IBPs, this type of processes require low inlet concentrations of contaminants, so it is the processes that need to reuse the regenerated stream. The processes with CPS value exceeding the average CPS value of all processes that need to be regenerated. According to the above discussion, the pre-regeneration subnetwork contains FOPs and OEPs, and the regeneration subnetwork contains IBPs.

#### 3.2 Design of subnetworks

Figure 1 is the design procedure of this work. The design of subnetworks is divided into six steps as shown in following subsections.

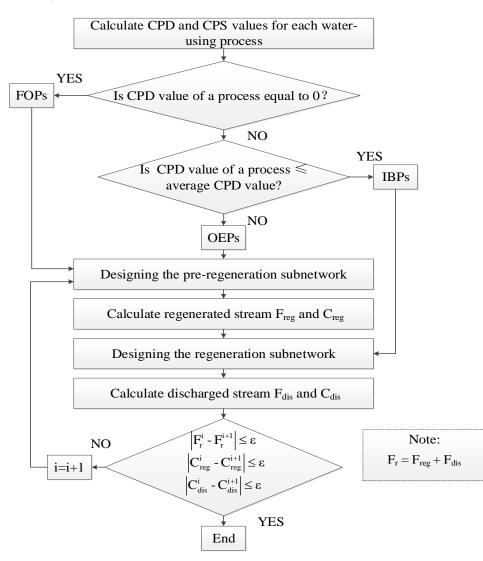


Figure 1: The design procedure

# 3.2.1 Step 1: Determine the initial value used for the iteration

For the first iteration, the limiting data of processes is used as the initial value. For the following iterations, the import and export concentrations of the processes obtained in the last iteration are used as initial values.

# 3.2.2 Step 2: Designing the pre-regeneration subnetwork

The water-using processes are performed in CPD ascending. The order of the source streams reused for water-using processes is internal source stream, regenerated stream, freshwater. When source streams are reused for water-using networks, the source stream with the largest  $R_{i,j}$  is reused first. If the internal source streams do not satisfy the process, the process needs to reuse the regenerated stream and/or fresh water.

# 3.2.3 Step 3: Calculation of regenerated stream

All the discharged water streams of the pre-regeneration subnetwork are mixed and then regenerated. Suitable regeneration unit(s) will be selected based on the inlet concentration of the IBP, when the IBP reuses the regenerated stream, the  $R_{i,j}$  value is greater than or equal to 1. At this time, the calculation result of the flowrate of regenerated stream is recorded as  $F_{reg}$  and the result of concentration is recorded as  $C_{reg}$ .

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#### 3.2.4 Step 4: Designing the regeneration subnetwork

In the regeneration network, regenerated streams can satisfy the IBP.

#### 3.2.5 Step 5: Calculation of water-using network discharge stream

The discharge streams of the regeneration subnetwork are mixed, and suitable regeneration unit(s) will be selected based on the mixed stream concentration and discharge limit. Flowrate and concentration of the WUN discharge stream can be calculated and recorded as  $F_{dis}$  and  $C_{dis}$ .

#### 3.2.6 Step 6: Record the iteration results of the water-using processes

According to the above five steps, the import and export concentrations and flowrates of all processes are obtained.  $F_{dis}$  and  $C_{dis}$  have also obtained. These data will be used as the initial value for the next iteration. It is also worth noting that both the regenerated stream in the third step and the discharge stream in the sixth step pass through the regeneration unit(s). Both  $F_{reg}$  and  $F_{dis}$ need to be counted when calculating the flowrate of streams through the regeneration units ( $F_r$ ). Go to first step, iteration will be completed when the differences of  $F_{r,}$   $C_{reg}$  and  $C_{dis}$  in twice neighbor iterations are within 0.01ppm.

### 4. Case Study

The case is taken from Faria and Bagajewicz (2011). The limiting data are listed in Table 1 and RR values of are listed in Table 2. The discharge limits of contaminant A, B and C in this WUN are (20, 5, 100) ppm.

Process	Contaminant	C <sup>lim</sup> (ppm)	C <sup>lim</sup> (ppm)	M <sub>reg</sub> (kg/h)
P1	А	0	15	0.75
	В	0	400	20
	С	0	35	1.75
P2	А	20	120	3.4
	В	300	12500	414.8
	С	45	180	4.59
P3	А	120	220	5.6
	В	20	45	1.4
	С	200	9500	520.8
P4	А	0	20	0.16
	В	0	60	0.48
	С	0	20	0.16
P5	А	50	150	0.8
	В	400	8000	60.8
	С	60	120	0.48

Table 1: The Limiting Data for Example From Faria and Bagajewicz (2011)

Contaminant	Removal Ratio of Unit 1 (%)	) Removal Ratio of Unit 2 (%	) Removal Ratio of Unit 3 (%)
A	0	70	95
В	99.9	90	0
С	0	98	50

Procedure for division of networks: CPD and CPS values for P1 to P5 can be calculated according to Table 1. It can be obtained from Table 3, the CPD values of P1 and P4 are equal to 0, therefore, P1 and P4 are FOPs. The CPD value of P3 is lower than average CPD value, P3 is IBP. The remaining P2 and P5 are OEPs and their CPS values are higher than the average CPS value. The pre-regeneration subnetwork contains FOPs and OEPs, while the regeneration subnetwork contains IBP.

Table 3: CPD and CPS	values for P1	to P5
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	P1	P2	P3	P4	P5	Average Value
CPD	0	1.816	0.408	0	3.588	1.163
CPS	0.556	17.361	31.148	0.261	11.111	7.322

In the first iteration, the procedure for design of subnetworks is as follows: The processes in the preregeneration subnetwork (FOPs and OEPs) are arranged in CPD ascending order. CPD can be obtained from the limiting data of FOPs (P1 and P4) and OEPs (P2 and P5). P1 and P4 are performed first, they use freshwater 50 t/h and 8 t/h. CPD value of P2 is 1.812 and CPD of P5 is 3.582. Then, P2 is performed. When  $S_1$  and  $S_4$  are reused for  $D_2$ , the  $R_{i,j}$  value are 0.93 and 1, the consumption are 24.3 t/h and 8 t/h. Since  $S_1$ and  $S_4$  cannot satisfy  $D_2$ ,  $D_2$  needs to reuse 1.7 t/h freshwater. Now, P5 is performed, and 8 t/h of  $S_1$  can be used. From above calculation, 34 t/h of  $S_2$ , 8 t/h of  $S_5$  and 17.7 t/h of  $S_1$  are mixed to pass through the regeneration unit 1. The  $F_{reg}$  is 59.7 t/h, and  $C_{reg}$  is (85.89, 8.31, 116.92) ppm. The water-using processes in the regeneration subnetwork is IBP (P3), and the source stream contains only the  $F_{reg}$ . When  $F_{reg}$  is reused for  $D_3$ , the  $R_{i,j}$  value is 1.42, and  $F_{reg}$ =55.51 t/h. 55.51 t/h of  $S_3$  and 4.19 t/h of  $F_{reg}$  are mixed to pass through the regeneration unit 2 and 3. It can be obtained that the  $F_{dis}$  is 59.7 t/h, and  $C_{dis}$  is (2.69, 3.18, 88.41) ppm. The first iteration is finished, the inlet and outlet concentrations and flowrates of P1 to P5,  $F_{dis}$  and  $C_{dis}$  will be used as the initial value for the second iteration. In the second iteration,  $F_{dis}$  is used as a source stream to reuse for P2. 1.7 t/h of  $F_{dis}$  replaces freshwater and minimizes the consumption of freshwater.

The following iterations can be completed similarly as discussed above, and the results for iteration 1 to 4 are shown in Table 4. The difference between the third and the fourth iteration is within 0.01 ppm, therefore, the calculation process can be finished with four iterations. And design results of this example is shown in Figure 2.

Iteration		1	2	3	4
F <sub>fresh</sub> (t/h)		59.7	58	58	58
F <sub>reg</sub> (t/h)		59.7	59.7142	59.7142	59.7142
F <sub>dis</sub> (t/h)		119.4	119.4284	119.4284	119.4284
Fr (t/h)		179.1	179.1426	179.1426	179.1426
C <sub>reg</sub> (ppm)	А	85.59464	85.65153	85.65383	85.65383
	В	8.309548	8.307663	8.307666	8.307666
	С	116.9179	119.4279	119.5031	119.5031
C <sub>dis</sub> (ppm)	А	2.690955	2.771021	2.771056	2.771056
	В	3.176013	3.269113	3.269113	3.269113
	С	88.40536	91.02268	91.02345	91.02345

Table 4: Calculation Results for the Case

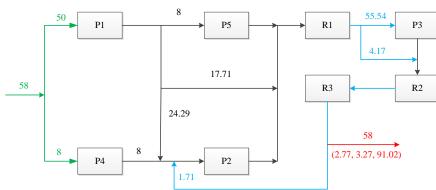


Figure 2: Design results of Example

For this example, the results obtained with different methods are listed in Table 5, where total IC is total interconnections. The consumption of freshwater is 58t/h, which has reached the minimum, and the results of freshwater consumption are the same as results in the literature. The consumption of regenerated water is 179.143 t/h, which has reduced by 60 t/h compared to the literature. The results of regenerated water consumption in this work are 25% lower than the results in the literature. The total IC is 11, which has reduced by one compared to the results of the literature.

In summary, the design method of this work reduces the consumption of regenerated water compared with the literature method.

Table 5: Comparison of different methods for the case study

	This Work	Faria and Bagajewicz (2011)
F <sub>fresh</sub> , t/h	58	58
F <sub>r</sub> , t/h	179.143	239.867
Total IC	11	12

# 5. Conclusions

An Iterative and Subnetwork-Dividing method is introduced in this work, the method can be used for the design of WUNs with multiple regeneration units. This paper investigates an example involving regeneration recycling, in the design procedure, freshwater consumption is minimized and the flowrates of regenerated stream is reduced by 25%. And it can be seen from the Table 5, the results obtained in this study are comparable to that obtained in the literature. The combination of multiple methods can make the design of water-using network more reasonable. Hence, for future work, the combination of another water-using network design method (such as mathematical programming) and the method proposed in this article should be paid more attention.

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