A Numerical-Indicator-Based Method for Design of Distributed Wastewater Treatment Systems with Multiple Contaminants

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In the design of distributed wastewater treatment systems with multiple contaminants, it is very important to minimize unnecessary stream mixing to reduce total treatment flow rate as much as possible. A new numerical indicator, total mixing influence potential (TMIP), to reflect the influence of the stream mixing caused by performing a process on the total treatment flow rate of a distributed wastewater system is introduced. In design procedure, the TMIP value is calculated based on pinch principle. The process with the smallest TMIP value will be performed first. The results of a few literature examples show that designs with very low (even minimum) total treatment flow rates can be obtained with the method proposed. In addition, the method proposed is simple and of clear engineering insight. The calculation effort does not increase significantly when the number of streams, contaminants, and/or treatment units increases. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 3223–3231, 2015
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Introduction

Wastewater treatment system integration, which is one of the important aspects in water resource management, has received more and more attention in the past two decades due to the increasing wastewater discharge and the more stringent environmental regulations. In a distributed treatment system, wastewater streams are primarily segregated for treatment and only mixed where appropriate. Therefore, the total treatment flow rate of a distributed treatment system can be reduced significantly, compared to that of a traditional centralized treatment system which mixes all the streams together before treatment.[1–5]

The integration of distributed wastewater treatment system can be mainly achieved by pinch analysis approaches and mathematical programming approaches. In 1994, Wang and Smith[4] first introduced pinch analysis approach for design of distributed wastewater treatment systems. The minimum treatment flow rate target was identified by graphical method, and then several rules based on pinch location were proposed to develop a design to realize the target. Kuo and Smith[5] presented an improved method of Wang and Smith,[4] which will be discussed in detail later. Kuo and Smith[6] further studied the interactions between design of water reuse and effluent treatment, and developed a methodology to explore design options which took into account the interactions. Ng et al.[7,8] presented a targeting procedure for the total water system consisting of water reuse, regeneration, and wastewater treatment, and investigated the interactions among different elements of the system using graphical and algebraic approaches. Soo et al.[9] extended the targeting procedure proposed by Ng et al.[8] to multi-treatment-unit systems with one- or two-contaminant. Bandyopadhyay[10] used an algebraic and graphical method to target the minimum treatment flow rate for the systems with flow loss. Liu et al.[11] presented an analytical method for wastewater treatment systems with single contaminant based on pinch stream identification. The pinch approaches discussed above are commonly used to design single or simple multicontaminant systems.

Mathematical programming approaches are the main tools for complex wastewater treatment system integration. In 1980, Takama et al.[12] initiated the research on water allocation problem using mathematical optimal approach. They presented a superstructure consisting of water-using units and wastewater treatment units and solved the resulted nonlinear problem by

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introducing a complicated penalty function. Galan and Grossmann[13,14] proposed a successive relaxed solution to solve nonconvex nonlinear problem for design of multicontaminant wastewater treatment networks (WTNs). Hernandez-Suarez et al.[15] employed superstructure decomposition and parametric optimization strategies for synthesis of the distributed treatment networks with no stream recycle or recirculation. Martín-Sistac and Graells[16] presented a simplified problem formulation for distributed wastewater systems and introduced a hybrid search procedure for solving the model. Liu et al.[17] introduced a particle swarm optimization method without relying on initial points for design of WTN. Statyukha et al.[18] built a superstructure based on pinch analysis and wastewater degradation concept and presented a simple but robust optimization algorithm. Castro et al.[19,20] adopted two-stage strategies for optimal design of wastewater treatment systems. The first stage generates good starting points with a linear programming formulation for the solution of the nonlinear programming of the second stage. Teles et al.[21] presented a new global optimization approach for design of water-using and wastewater treatment subsystems using multiparametric disaggregation strategies. Burgara-Montero et al.[22] developed a multiobjective programming model and solved it by a discretization optimal approach. Saif et al. addressed optimal design of reverse-osmosis (RO) WTNs[23] and split partial second pass RO networks for desalination application[24] through superstructure optimization. Karuppiah et al.[25] also addressed the problem of optimal design of RO water treatment systems with a superstructure optimization method. Park et al.[26] considered the eco-designs of the existing wastewater treatment systems which optimized the trade-offs between the environmental impacts and economic costs. Alnouri et al.[27] presented integration strategies for optimal design of interplant water networks within an industrial city, in which centralized and decentralized water treatment options were introduced. Apart from the above works on the separate wastewater treatment problem, some researchers extended the study scope to the total water system[28–35] and complete water system.[36,37] The designs obtained can further reduce the freshwater consumption, wastewater treatment amount, and total costs. Correspondingly, the superstructures are more complex and the model solutions are more difficult. In a word, a lot of efforts have been made to solve the nonlinear programming models of distributed wastewater treatment superstructures. However, with the increase of the number of streams, contaminants, and/or treatment units, the problem sizes usually grow significantly. It is difficult to obtain the global optimal solution even feasible solution sometimes.

Now, we discuss the work of Kuo and Smith[5] in detail. In their work, to target and design distributed wastewater systems with multiple contaminants, a set of subnetworks for each individual contaminant were designed first and then were merged reasonably to obtain the final design for all contaminants. By analysis, they addressed that each subnetwork incorporated some degradation which could result in increasing of treatment flow rates in the downstream processes. To measure the extent of wastewater degradation, they introduced the concept of mixing exergy loss. This concept provides valuable insights into design of distributed treatment systems with multiple contaminants, but it is generally applicable to the simple systems. Shi and Liu[38] proposed a new concept, total treatment flow rate potential (TTFP), which can reflect a measurement of the minimum total treatment flow rate of a process to remove a contaminant to meet the environmental limit. In design of a treatment system, the process with the minimum TTFP value was performed first. However, in some cases, the value of TTFP obtained cannot reflect the minimum total treatment flow rate properly, especially when the concentration(s) of some contaminant(s) is very small. Liu et al.[39] presented a few heuristic rules to reduce unnecessary stream mixing in determining process sequence for distributed treatment systems with multiple contaminants. However, it is difficult to determine process sequence when dealing with complex systems, due to the lack of a specific quantitative index.

McLaughlin et al.[40] pointed out that in most cases, capital and operating costs of a treatment network are proportional to the wastewater amounts flowing through the treatment units. In addition, for a given mass load of contaminant, the costs increase with the decreasing concentration which can result in the reduction of the process driving force. In design of a distributed treatment system, it is unnecessary stream mixing caused by performing a process that reduces the concentrations of contaminants, and thus increases the treatment flow rates of the downstream processes. Therefore, it is very important to avoid unnecessary stream mixing as much as possible. To minimize stream mixing, it is essential to measure stream mixing quantitatively and properly. In this article, we will introduce a new numerical indicator to reflect the influence of the stream mixing caused by performing a process on the total treatment flow rate of the system. The process sequence will be then determined based on the numerical indicator. In the design procedure, the value of the numerical indicator is calculated based on pinch principle. Finally, a few literature examples will be investigated to show the method proposed.

Problem Statement

Given are a set of effluent streams with certain flow rates, in which a few contaminants with certain concentrations need to be removed to meet the environmental regulations. Given are also a set of treatment processes, which are not constrained by the maximum inlet concentration limits, each can remove a subset of contaminants with certain removal ratio (RR_i). The objective of this work is to reduce the total treatment flow rate of the system by determining the reasonable process sequence, and reduce the number of the treatment processes as much as possible. It is assumed that there is no wastewater loss during treatment operating.

The New Method

This section is divided into four subsections. First, obtain the minimum treatment flow rate of a process. Second, introduce a new concept to evaluate the influence of the stream mixing caused by performing a process on the downstream processes. In the third subsection, we will propose a numerical indicator to reflect the influence of performing a process on the total treatment flow rate, and determine the performing sequence of the processes. Finally, the design procedure will be proposed.

The minimum treatment flow rate of a process for its main contaminant

If a process can only remove one contaminant, the design procedure is simple. If a process can remove more than one contaminant, the contaminant corresponding to the maximum RR value is called as the main contaminant of the process.[39] The minimum treatment flow rate of a process for its main contaminant can be obtained with the pinch method proposed by Liu et al.,[11,39] which is sketched as follows.

Let us consider the situation when a contaminant, say contaminant A, is the main contaminant of treatment process TP_j, without considering the influence of other contaminants and processes. Arrange the wastewater streams according to the descending order of concentration of contaminant A, from S_1 to S_{NS}, where NS is the number of the streams. If some streams are of the same concentration, we arrange them according to the descending order of flow rate, because this sorting way can reduce stream mixing in the design procedure.

The minimum removal mass load of contaminant A is

$$M_A^{rem} = \sum_{i=1}^{NS} m_{i,A} - c_{env,A}^{lim} \times \sum_{i=1}^{NS} f_i \tag{1}$$

Accordingly, the mass load of contaminant A in the inlet stream of TP_j is

$$M_{TP_j,A} = M_A^{rem} / RR_A \tag{2}$$

where $m_{i,A} = f_i c_{i,A}, f_i$ is the flow rate of stream S_i, $c_{i,A}$ and $m_{i,A}$ are the concentration and mass load of contaminant A in S_i, $c_{env,A}^{lim}$ is the environmental limit concentration of contaminant A, and RR_A is the removal ratio of TP_j for contaminant A.

If the condition of formula 3 is met, stream S_p is the pinch stream, which should be partially treated and partially bypassed

$$\sum_{i=1}^{p-1} m_{i,A} < M_{TP_j,A} \le \sum_{i=1}^{p} m_{i,A} \tag{3}$$

The treatment flow rate of $S_p, f_{TP_j,pt}$, is

$$f_{TP_j,pt} = \frac{M_{TP_j,A} - \sum_{i=1}^{p-1} m_{i,A}}{c_{p,A}} \tag{4}$$

The bypassing flow rate of $S_p, f_{TP_j,pb}$, is

$$f_{TP_j,pb} = f_p - f_{TP_j,pt} \tag{5}$$

The streams that should be treated by TP_j are: S_1, S_2, ., S_{p-1} and part of S_p. The minimum treatment flow rate of TP_j is

$$f_{TP_j} = f_{TP_j,pt} + \sum_{i=1}^{p-1} f_i \tag{6}$$

Evaluating the influence of stream mixing caused by performing a process on the downstream processes

In this subsection, we will introduce a new concept to evaluate the influence of the stream mixing caused by performing a process on the downstream processes. When TP_j is performed, the streams which should be treated and the minimum treatment flow rate of TP_j can be obtained with Eqs. 1–6. Then, the streams after TP_j (as shown in Figure 1) are: S_m, S_{pb}, S_{p+1}, ..., S_{NS}, where S_m is the mixed stream with flow rate of f_{TP_j}, and S_{pb} is the bypassing portion of S_p with flow rate of $f_{TP_j,pb}$.

Based on the streams after TP_j shown in Figure 1, we can calculate the minimum treatment flow rate for a downstream process, say TP_k, to remove its main contaminant, say contaminant B. The minimum treatment flow rate of TP_k obtained may reflect the influence of the stream mixing caused by performing TP_j on the treatment flow rate of downstream process TP_k (hereafter referred to as: the influence of TP_j on TP_k). We define the minimum treatment flow rate of TP_k as the mixing influence treatment flow rate (MITF) of TP_j on TP_k, and denote it as $MI_{j,k}$.

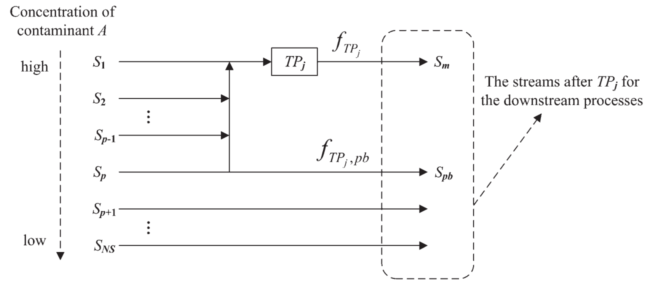

Figure 1. Streams after TP_j for the downstream processes.

Numerical indicator: Total mixing influence potential

Based on the discussions in the two previous subsections, we can obtain the minimum treatment flow rate and the MITF values for each process, which can form an MITF matrix as shown in formula 7, where NT is the number of the treatment processes. In the jth column vector of the MITF matrix, the element f_{TP_j} is the minimum treatment flow rate of TP_j, and the other elements reflect the influence of performing TP_j on its downstream processes. Therefore, the sum of all the elements in the jth column vector of the MITF matrix, MI_j, calculated by Eq. 8, can reflect the influence of the stream mixing caused by performing TP_j on the total treatment flow rate of the system. We define MI_j as the *total mixing influence potential* (TMIP) of process TP_j

$$\begin{bmatrix} f_{TP_1} & \cdots & MI_{j,1} & \cdots & MI_{NT,1} \\ \vdots & & \vdots & & \vdots \\ MI_{1,j} & \cdots & f_{TP_j} & \cdots & MI_{NT,j} \\ \vdots & & \vdots & & \vdots \\ & \cdots & MI_{j,k} & \cdots & \\ \vdots & & \vdots & & \vdots \\ MI_{1,NT} & \cdots & MI_{j,NT} & \cdots & f_{TP_{NT}} \end{bmatrix} \tag{7}$$

$$MI_j = \sum_{i=1}^{NT} MI_{j,i} \tag{8}$$

The smaller the TMIP value of a process, the less the influence of the stream mixing caused by performing the process on the total treatment flow rate. *Therefore, the process with the smallest TMIP value, say TP_q, should be performed first with the flow rate of f_{TP_q}*. This will reduce the total treatment flow rate of the system.

Design procedure

In the light of the above analysis, the design procedure is proposed as shown in Figure 2.

Case Studies

Example 1

The stream and treatment process data for Example 1 are shown in Table 1, taken from Kuo and Smith.[5] The environmental limit for each contaminant is 100 ppm.

The design procedure is as follows.

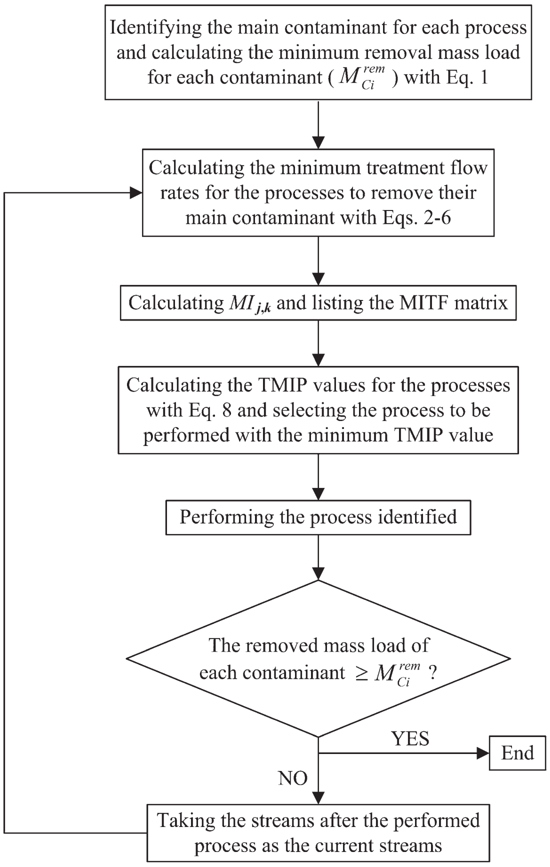

Figure 2. Design procedure proposed.

1. Identifying the main contaminant and calculating the minimum treatment flow rate for each process

   Let us take process TP_1 as an example. Process TP_1 only removing contaminant A, as shown in Table 1b, this contaminant is certainly the main contaminant of TP_1. Arrange all the streams according to the descending order of the concentration of contaminant A, as shown in Table 2. The minimum removal mass load of contaminant A is $19,000-40\times100=15,000$ g/h, according to Eq. 1 and the data in Table 2. The mass load of contaminant A in the inlet stream of TP_1 is $15,000/0.9=16,667$ g/h from Eq. 2. Because $12,000$ g/h $<16,667$ g/h $<18,000$ g/h (see Table 2), according to formula 3, S_2 is the pinch stream of TP_1. The treatment flow rate of S_2 is $(16,667-12,000)/400=11.67$ t/h from Eq. 4. Therefore, the minimum treatment flow rate of TP_1 is $20+11.67=31.67$ t/h, according to Eq. 6. Similarly, the minimum treatment flow rate of other processes can be obtained, as listed in Table 3.

Table 1. Data for Example 1

(a) Stream Data

Stream	Concentration (ppm) A	B	C	Flow Rate (t/h)
S_1	600	500	500	20
S_2	400	200	100	15
S_3	200	1000	200	5

(b) Treatment Process Data

Process	Removal Ratio (%) A	B	C
TP_1	90	0	0
TP_2	0	99	0
TP_3	0	0	80

Table 2. Calculation of the Minimum Treatment Flow Rate of TP_1 for Example 1

Stream	$c_{i,A}$ (ppm)	f_i (t/h)	$m_{i,A}$ (g/h)	$\Sigma m_{i,A}$ (g/h)	f_{TP_1} (t/h)
S_1	600	20	12,000	12,000	20
S_2	400	15	6000	18,000	11.67
S_3	200	5	1000	19,000	
Sum	–	40	19,000	–	31.67

Table 3. The Minimum Treatment Flow Rate of Each Process for Example 1

Process	Main Contaminant	M_{Ci}^{rem} (g/h)	Streams Treated	f_{TP_j} (t/h)
TP_1	A	15,000	S_1, S_2	31.67
TP_2	B	14,000	S_3, S_1	23.28
TP_3	C	8500	S_1, S_3	23.13

2. Determining the first process to be performed

   Calculate the MITFs for each process first. We will take the detailed calculation of $MI_{1,2}$ as an example. When TP_1 is performed, the streams after TP_1 shown in Figure 3 are: S_{m1}, which is mixed by S_1 and part of S_2 with the flow rate of 31.67 t/h; S_{2b}, which is the bypassing portion of pinch stream S_2 with the flow rate of $15-11.67=3.33$ t/h; and S_3. Rearrange these streams according to the descending order of the concentration of contaminant B, which is the main contaminant of TP_2, as shown in Table 4, where the concentration of contaminant B in S_{m1} is $(20\times500+11.67\times200)/31.67=389.45$ ppm. Based on Eqs. 1–6 and the stream data shown in Table 4, we can obtain that the minimum treatment flow rate of TP_2 is 28.47 t/h, which is listed in the last column of Table 4. According to the definition of the MITF, the value of $MI_{1,2}$ is 28.47 t/h. Similarly, the other MITFs can be obtained.

   The MITF matrix is shown in Eq. 9

$$\begin{bmatrix} f_{TP_1} & MI_{2,1} & MI_{3,1} \\ MI_{1,2} & f_{TP_2} & MI_{3,2} \\ MI_{1,3} & MI_{2,3} & f_{TP_3} \end{bmatrix} = \begin{bmatrix} 31.67 & 34.17 & 33.23 \\ 28.47 & 23.28 & 23.49 \\ 30.13 & 24.14 & \mathbf{23.13} \end{bmatrix} \tag{9}$$

   The TMIP values for the processes calculated with Eq. 8 are as follows

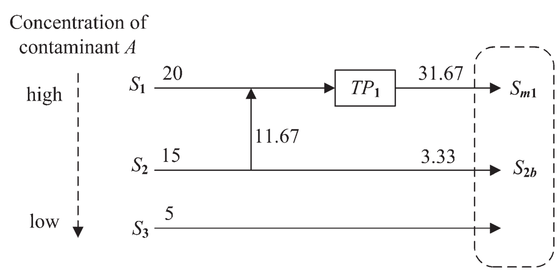

Figure 3. Streams after TP_1 for the downstream processes of Example 1.

Table 4. Calculation of $MI_{1,2}$ for Example 1

Streams after TP_1	$c_{i,B}$ (ppm)	f_i (t/h)	$m_{i,B}$ (g/h)	$\Sigma m_{i,B}$ (g/h)	$MI_{1,2}$ (t/h)
S_3	1000	5	5000	5000	5
S_{m1}	389.45	31.67	12,333.88	17,333.88	23.47
S_{2b}	200	3.33	666	17,999.88	
Sum					28.47

$$[MI_1 \quad MI_2 \quad MI_3] = [90.27 \quad 81.59 \quad 79.85] \tag{10}$$

It can be seen from Eq. 10 that the TMIP value of TP_3 is the smallest. Therefore, TP_3 should be performed first with the flow rate of 23.13 t/h, which is the element of f_{TP_3} in Eq. 9, and printed in bold.

3. Determining the second process to be performed
   The current stream data after TP_3 are shown in Table 5. Based on the data in Table 5, we can obtain the MITF matrix for TP_1 and TP_2, as shown in Eq. 11

$$\begin{bmatrix} f_{TP_1} & MI_{2,1} \\ MI_{1,2} & f_{TP_2} \end{bmatrix} = \begin{bmatrix} 33.23 & \mathbf{34.17} \\ 28.79 & \mathbf{23.49} \end{bmatrix} \tag{11}$$

The TMIP values for TP_1 and TP_2 calculated with Eq. 8 are as follows

$$[MI_1 \quad MI_2] = [62.02 \quad 57.66] \tag{12}$$

Therefore, the second process to be performed is TP_2 and the last one is TP_1. The flow rates of TP_2 and TP_1 are 23.49 and 34.17 t/h, which are printed in bold in Eq. 11.

The total treatment flow rate is 80.79 t/h and the final design is shown in Figure 4. The design obtained by this work is the same as the optimal design of Kuo and Smith,[5] and agrees with that obtained by Shi and Liu[38] and Liu et al.[39] However, it can be seen from the above design procedure that the process sequence and flow rates of the treatment units can be obtained simultaneously. Therefore, the method proposed in this article is simple, compared to the literature methods.

Example 2

The stream and treatment process data for Example 2 taken from Castro et al.[19] are shown in Table 6. The environmental limit for each contaminant is 100 ppm.

The design procedure is as follows.

1. Identifying the main contaminant and calculating the minimum treatment flow rate for each process
   Process TP_1, TP_2, and TP_3 can only remove contaminant *A*, *B*, and *C*, respectively, as can be seen from Table 6b. Process TP_4 can remove two contaminants, *D* and *E*, with the removal ratios of 99 and 90%, respectively. Therefore, the main contaminant of TP_4 is *D*. Because it is unnecessary to consider contaminant *F* whose mass loads in all streams are less than the environmental limit mass load, as can be seen from Table 6a, the main contaminant of TP_5 is *E*.
   The minimum treatment flow rate for each process to remove its main contaminant can be calculated with Eqs. 1–6 and the results are shown in Table 7.

Table 5. Current Stream Data After TP_3 for Example 1

Current Stream	Concentration (ppm) *A*	*B*	Flow Rate (t/h)
S_{m1}	545.87	567.66	23.13
S_{3b}	200	1000	1.87
S_2	400	200	15

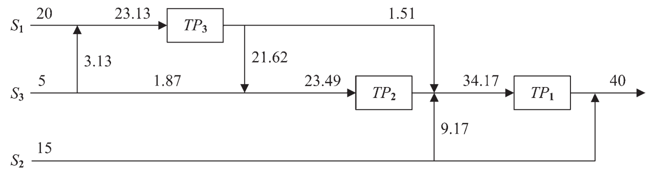

Figure 4. Design for Example 1 (where the numbers are flow rates in t/h).

2. Determining the first process to be performed
   The MITF matrix is as follows

$$\begin{bmatrix} 27.96 & 33.06 & 30.38 & 31.51 & 38.19 \\ 27.73 & 23.13 & 23.14 & 23.13 & 35.89 \\ 27.27 & 21.82 & \mathbf{21.82} & 21.82 & 34.77 \\ 32.06 & 30.02 & 30.02 & 30.02 & 33.92 \\ 43.71 & 43.81 & 43.76 & 49.41 & 43.71 \end{bmatrix} \tag{13}$$

The TMIP values for the processes calculated with Eq. 8 are as follows

$$[158.73 \quad 151.84 \quad 149.12 \quad 155.89 \quad 186.48] \tag{14}$$

It can be seen from formula 14 that the TMIP value of TP_3 is the smallest. Therefore, TP_3 should be performed first with the flow rate of 21.82 t/h, which is printed in bold in Eq. 13.

3. Determining the second process to be performed
   The MITF matrix for TP_1, TP_2, TP_4, and TP_5 is

$$\begin{bmatrix} 30.36 & 33.06 & 33.74 & 39.69 \\ 27.69 & \mathbf{23.14} & 23.14 & 23.14 \\ 32.09 & 30.02 & 30.02 & 33.92 \\ 43.83 & 43.81 & 43.76 & 43.76 \end{bmatrix} \tag{15}$$

Table 6. Data for Example 2

(a) Stream Data

Stream	Concentration (ppm) *A*	*B*	*C*	*D*	*E*	*F*	Flow Rate (t/h)
S_1	1100	500	500	200	800	100	19
S_2	40	0	100	300	910	200	7
S_3	200	220	200	500	150	0	8
S_4	60	510	500	200	780	100	6
S_5	400	170	100	300	900	0	17

(b) Treatment Process Data

Process	Removal Ratio (%) *A*	*B*	*C*	*D*	*E*	*F*
TP_1	99					
TP_2		99				
TP_3			99			
TP_4				99	90	
TP_5					99	99

Table 7. The Minimum Treatment Flow Rate of Each Process for Example 2

Process	Main Contaminant	M_{Ci}^{rem} (g/h)	Streams Treated	f_{TP_j} (t/h)
TP_1	A	24,240	S_1, S_5	27.96
TP_2	B	11,510	S_4, S_1	23.13
TP_3	C	10,800	S_1, S_4	21.82
TP_4	D	10,500	S_3, S_5, S_2	30.02
TP_5	E	37,050	S_2, S_5, S_1, S_4	43.71

The TMIP values for TP_1, TP_2, TP_4, and TP_5 calculated with Eq. 8 are as follows

$$[\,133.97 \quad 130.03 \quad 130.66 \quad 140.51\,] \tag{16}$$

It can be seen from formula 16 that TP_2, with the smallest TMIP value, should be the second process to be performed. The flow rate of TP_2 is 23.14 t/h, which is printed in bold in Eq. 15.

4. Determining the third process to be performed

The MITF matrix for TP_1, TP_4, and TP_5 is

$$\begin{bmatrix} \mathbf{33.06} & 36.26 & 41.96 \\ 32.07 & 30.02 & 33.93 \\ 43.97 & 49.41 & 43.81 \end{bmatrix} \tag{17}$$

The TMIP values for TP_1, TP_4, and TP_5 calculated with Eq. 8 are as follows

$$[\,109.10 \quad 115.69 \quad 119.70\,] \tag{18}$$

Therefore, the third process to be performed is TP_1 with the flow rate of 33.06 t/h, which is printed in bold in Eq. 17.

5. Determining the forth process to be performed

Now, there are two processes left: TP_4 and TP_5. Process TP_4 should take precedence over TP_5 because TP_4 can remove contaminants D and E, while TP_5 can only remove contaminant E. If TP_4 is capable of removing M_E^{rem} (37,050 g/h, in Table 7) completely, TP_5 is unnecessary to be performed; if not, TP_5 is required to remove the remaining mass load of contaminant E. From the current stream data after TP_1 shown in Table 8, the flow rate of TP_4 can be obtained as 32.07 t/h, and the mass load of contaminant E removed by TP_4 is 20,059.21 g/h. Then, the mass load to be removed by TP_5 is $37,050-20,059.21 = 16,990.79$ g/h. The flow rate of TP_5 can be obtained as 20.91 t/h.

The total treatment flow rate, f_{total}, is 131.00 t/h and the final network structure is shown in Figure 5. Table 9 compares this design with those in the literature.

Table 8. Current Stream Data After TP_1 for Example 2

Current Stream	Concentration (ppm)		Flow Rate (t/h)
	D	E	
S_{m3}	224.39	820.76	33.06
S_{5b}	300	900	8.94
S_3	500	150	8
S_2	300	910	7

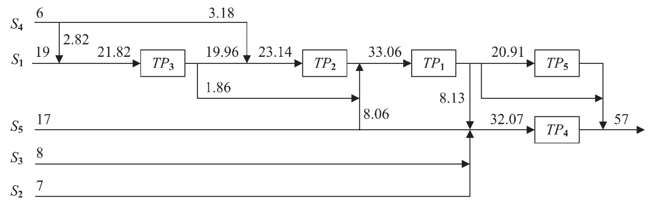

Figure 5. Design for Example 2 (where the numbers are flow rates in t/h).

Compared to the design of Liu et al.,[39] the total treatment flow rate of this work is reduced by 2.78%, with the interconnection number being similar. Compared to the design of Castro et al.[20] and Teles et al.,[21] the total treatment flow rate of this work increases by 5.27%, with the interconnection number being the same. However, there is no low-flow rate stream (<1.5 t/h) in the design of this work. In addition, it can be seen from the above design procedure that when the number of streams, contaminants, and/or treatment units increases, the calculation effort of the proposed method does not increase apparently.

Example 3

The stream and treatment process data taken from Galan and Grossmann[14] are shown in Table 10. There are 15 effluent streams with significant difference in contaminant concentrations. Treatment processes except TP_3 can remove two contaminants. Therefore, this system is relatively complex. The environmental limit for each contaminant is 100 g/m^3.

The design procedure is as follows.

1. Identifying the main contaminant and calculating the minimum treatment flow rate for each process

Identify the main contaminant for each process. It should be noted that for TP_5, although the RR value for contaminant E is higher than contaminant B, its main contaminant is contaminant B, because that there is no process whose main function is to remove contaminant B. The minimum treatment flow rate for each process to remove its main contaminant can be calculated and the results are shown in Table 11.

It can be seen from Table 11 that TP_3, which only removes contaminant E, is the process that can lead to the maximum mixing. Meanwhile, TP_4 and TP_5 can also remove contaminant E with RR values of 90 and 99%, apart from their respective main contaminants. Therefore, TP_3, which cannot be performed first, is unnecessary to be considered for the moment.

Table 9. Comparison of the Results for Example 2

Literature	f_{total} (t/h)	Interconnection Number	Other
This work	131.00	15	The minimum flow rate is 1.86 t/h
Liu et al.[39]	134.75	14	The minimum flow rate is 1.87 t/h
Castro et al.[20]	124.44	15	Three low-flow rate streams included (<1.5 t/h)

Table 10. Data for Example 3

(a) Stream Data

Stream	Concentration (g/m^3) A	B	C	D	E	Flow Rate (m^3/s)
S_1	100	50	350	0	70	36
S_2	600	800	1500	0	910	24
S_3	900	0	600	150	230	15
S_4	10	10	100	3000	850	25
S_5	40	170	0	500	690	18
S_6	0	1100	0	200	340	35
S_7	120	10	500	2000	70	9
S_8	370	20	100	30	690	2
S_9	900	350	200	80	230	3
S_{10}	250	270	90	0	580	23
S_{11}	0	1190	60	230	370	89
S_{12}	0	0	20	800	100	1
S_{13}	2000	600	340	0	30	5
S_{14}	0	5	100	600	40	41
S_{15}	1000	1510	270	150	220	8

(b) Treatment Process Data

Process	Removal Ratio (%) A	B	C	D	E
TP$_1$	40		98		
TP$_2$	90	50			
TP$_3$					90
TP$_4$				99	90
TP$_5$		90			99

2. Determining the first process to be performed
   The MITF matrix for TP$_1$, TP$_2$, TP$_4$, and TP$_5$ is

$$\begin{bmatrix} 45.71 & 49.95 & 48.59 & 175.25 \\ 31.41 & 26.75 & 26.75 & 38.51 \\ 123.75 & 92.17 & \mathbf{92.17} & 92.17 \\ 175.10 & 169.18 & 155.83 & 155.83 \end{bmatrix} \tag{19}$$

The TMIP values for TP$_1$, TP$_2$, TP$_4$, and TP$_5$ are as follows

$$[375.97 \quad 338.05 \quad 323.34 \quad 461.76] \tag{20}$$

It can be seen from formula 20 that the TMIP value of TP$_4$ is the smallest. Therefore, TP$_4$ should be performed first with the flow rate of 92.17 m^3/s, which is printed in bold in Eq. 19.

Table 11. The Minimum Treatment Flow Rate of Each Process for Example 3

Process	Main Contaminant	M_{Ci}^{rem} (g/s)	Streams Treated	f_{TP_j} (m^3/s)
TP$_1$	C	47,390	S_2, S_3, S_7	45.71
TP$_2$	A	27,340	S_{13}, S_{15}, S_3	26.75
TP$_3$	E	92,600	S_2, S_4, S_5, S_8, S_{10}, S_{11}	180.27
TP$_4$	D	125,220	S_4, S_7, S_{12}, S_{14}, S_5	92.17
TP$_5$	B	157,995	S_{15}, S_{11}, S_6, S_2	155.83

Table 12. Discharged Concentration of Each Contaminant for Example 3

	Contaminant A	B	C	D	E
Mass load removed (g/s)	34,715	157,995	47,390	125,220	98,694
Discharged concentration (g/m^3)	77.92	100	100	100	81.75

3. Determining the second process to be performed
   The MITF matrix for TP$_1$, TP$_2$, and TP$_5$ is

$$\begin{bmatrix} 48.59 & 50.89 & 145.56 \\ 32.30 & \mathbf{26.75} & 38.51 \\ 176.65 & 169.18 & 155.83 \end{bmatrix} \tag{21}$$

The TMIP values for TP$_1$, TP$_2$, and TP$_5$ are as follows

$$[257.54 \quad 246.82 \quad 339.9] \tag{22}$$

It can be seen from formula 22 that TP$_2$, with the smallest TMIP value, should be the second process to be performed. The flow rate of TP$_2$ is 26.75 m^3/s, which is printed in bold in Eq. 21.

4. Determining the third process to be performed
   The MITF matrix for TP$_1$ and TP$_5$ is

$$\begin{bmatrix} \mathbf{50.89} & 138.57 \\ \mathbf{167.83} & 149.45 \end{bmatrix} \tag{23}$$

The TMIP values for TP$_1$ and TP$_5$ are as follows

$$[218.72 \quad 288.02] \tag{24}$$

Therefore, the third process to be performed is TP$_1$, and the fourth one is TP$_5$. The flow rates of TP$_1$ and TP$_5$ are 50.89 and 167.83 m^3/s, which are printed in bold in Eq. 23. After *TP*$_5$, the removed mass load for each contaminant has been equal to or greater than the corresponding minimum removal mass load, TP$_3$ is thus unnecessary to be performed. The removed mass load and the final discharge concentration

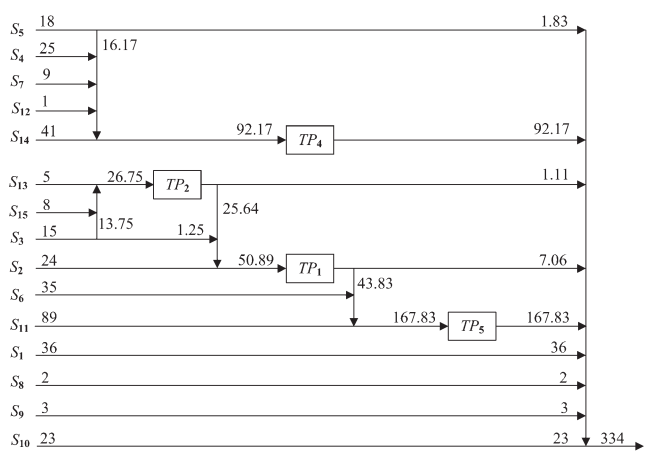

Figure 6. Design for Example 3 (where the numbers are flow rates in m^3/s).

Table 13. Comparison of the Results for Example 3

Literature	f_{total} (m^3/s)	Interconnection Number	Other
This work	337.64	23	Four streams bypass completely and one process unnecessary
Liu et al.[39]	381.19	23	Two streams bypass completely and one process unnecessary
Galan and Grossmann[14]	440	–	–

for each contaminant are listed in Table 12. Table 12 shows that the discharged concentrations of contaminants *A* and *E* are below their environmental limits.

The total treatment flow rate, f_{total}, is 337.64 m^3/s and the final design is shown in Figure 6. It can be seen that the design procedure of this example is simple. The comparison between the design obtained in this work and those in the literature is listed in Table 13. Table 13 shows that the total treatment flow rate, the interconnection number, the number of the treatment processes and the number of the bypassing streams obtained in this work are all equal to or better than those in the literature.

A few other WTN examples taken from Castro et al.[19,20] and Teles et al.[21] are solved using the method proposed as well (in which Ex 7 and Ex 9 correspond to Example 1 and Example 2 of this article). The final designs for these examples are given in the Supporting Information. The comparison of the results for Ex 2–8 in the literature[19–21] and those obtained in this work is shown in Table 14. It can be seen from Table 14 that the results obtained in this article are almost the same as those of Teles et al.,[21] which have been proved to be the global optimal solutions. Therefore, the proposed method could be generally applicable to the WTN problems without the maximum inlet concentration limits.

Discussion and Conclusions

A new method is presented for design of distributed wastewater treatment systems with multiple contaminants. It is unnecessary stream mixing caused by performing a process that leads to the increase of the treatment flow rates of the downstream processes. Based on this insight, we introduce a numerical indicator, *total mixing influence potential* (TMIP), to reflect the influence of performing a process on the total treatment flow rate of the system. The TMIP values, which can be calculated based on pinch principle, are used to identify the precedence order of the processes: the process with the smallest TMIP value is performed first. The results of a few literature examples show that the introduction of the numerical indicator provides an effective tool for design of the distributed wastewater treatment systems with multiple contaminants. The proposed method is simple and of clear engineering insight. In addition, the calculation effort does not increase significantly when the number of streams, contaminants, and/or treatment units increases.

As addressed in the section "Problem Statement," we mainly studied the WTN problems without the maximum inlet concentration limits to the treatment processes in this article. For the situation when some treatment processes are constrained by the maximum inlet concentration limits, we have presented a heuristic method that is the subject of another article submitted to a Chinese journal. The problems which require recycling to meet the environmental regulations will be investigated in our future work.

Table 14. Comparison of the Results of a Few Examples from Literature[19–21]

Example	f_{total} (t/h) Literature[19–21]	This Work
Ex 2	130.703	130.70
Ex 3	99.495	99.50
Ex 4	89.836	89.84
Ex 5	229.701	229.70
Ex 6	173.48	173.82
Ex 8	109.401	109.43

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Notation

c_A^{dis} = environmental discharge concentration of contaminant *A*
$c_{env,A}^{lim}$ = environmental limit concentration of contaminant *A*
f_{TP_j} = the minimum treatment flow rate of TP_j, as defined by Eq. 6
$f_{TP_j,pb}$ = bypassing flow rate of pinch stream *Sp* by TP_j, as defined by Eq. 5
$f_{TP_j,pt}$ = treatment flow rate of pinch stream *Sp* by TP_j, as defined by Eq. 4
M_A^{rem} = the minimum removal mass load of contaminant *A*, as defined by Eq. 1
$M_{env,A}^{lim}$ = environmental limit mass load of contaminant *A*
$M_{TP_j,A}$ = mass load of contaminant *A* in the inlet stream of TP_j, as defined by Eq. 2
$C_{i,A}$ = concentration of contaminant *A* in stream S_i
f_i = flow rate of stream S_i
$m_{i,A}$ = mass load of contaminant *A* in stream S_i
MI_j = value of the TMIP for TP_j, as defined by Eq. 8
$MI_{j,k}$ = value of the MITF reflecting the influence of TP_j on TP_k
MITF = mixing influence treatment flow rate
NC = number of contaminants
NS = number of streams
NT = number of treatment processes
RR*A* = removal ratio for contaminant *A*
S_i = stream *i*
S_m = mixed stream
S_p = pinch stream
S_{pb} = bypassing portion of pinch stream S_p
TMIP = total mixing influence potential
TP_j = treatment process *j*

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APPENDIX A:

The supporting information associated with this article may be found in the online version with the file name Designs for WTN problems of Exs 2-8 from Teles et al. (*Comput Chem Eng*. 2012;40:132–147.)

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