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Mixing Potential: A New Concept for Optimal Design of Hydrogen and Water Networks with Higher Disturbance Resistance

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During the last decade, the design methods of hydrogen and water networks have been improved greatly. Since the resulting network structure featuring minimum utility consumption is not unique, other properties such as disturbance resistance have drawn more and more attention. In this article, a novel concept, Mixing Potential, is proposed to improve the disturbance resistance ability of the networks in the design stage. This concept originates from measuring the concentration fluctuation of a single sink, and could be calculated by its graphical and algorithmic definition, respectively. In addition, a sufficient condition for minimizing the Mixing Potential of a single sink has been proved. Based on this sufficient condition, a graphical and its corresponding algorithmic method are proposed to design the hydrogen and water networks with minimum utility consumption. Literature examples illustrate that the disturbance resistance ability of the network can be improved by adjusting the satisfying order of sinks. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3762–3772, 2014

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Introduction

The design methodologies for water networks and refinery hydrogen networks have been improved greatly during the last decade. For the two kinds of networks, typical design methods involve mathematical programming approaches[1,2] and insight-based conceptual techniques.[3] The design objective is to obtain an efficient and operable network. For mathematical programming methods, the efficient aspect is directly achieved by setting economic[4] and environmental[5] objectives. Mathematical methods have also been developed for accessing and optimizing the operable aspect. The operable aspect can be accessed either by indicators such as flexibility index,[6,7] resilience index,[8,9] and robustness metrics[10] or by Monte Carlo simulation.[11] To optimize the network robustness under uncertainty, methods such as stochastic programming[12], fuzzy programming,[13,14] scenario-based mathematical programming[15–18] chance constrained programming[19] and robust optimization[20] have been used. Although the mathematical methods are effective in handling complicated problems, they suffer from the limitation of computational burden especially for the problems about operability. Furthermore, they cannot provide insightful understandings to the results.

At the meantime, the pinch-based design approaches are free of computational burden and easy to understand. Usually, the network integration process involves two stages: flow rate targeting and network design. The objective of flow rate targeting is to achieve the minimum utility consumption and the targeting approaches include hydrogen surplus diagram,[21] source composite curve,[22,23] material recovery pinch diagram,[24–26] and limiting composite curves.[27] Once the minimum utility consumption determined, the network can be designed by these methods such as: load table,[28] source sink mapping diagram,[29] nearest neighbor algorithm (NNA),[27,30] and concentration potential method.[31] Recently, some researchers proposed the graphical methods to simultaneously target and design hydrogen and water networks, such as generic graphical technique,[32] process-based graphical approach,[33] and evolutionary graphical approach.[26] Although all these proposed approaches can be used to obtain hydrogen and water networks with minimum utility consumption, the operability of the achieved networks have not been considered yet.

Operability is often referred to as the ease with which a process is operated and controlled. In this article, we focus on a certain aspect of the operability problem, the disturbance resistance ability of the network. A new concept, Mixing Potential, is proposed to deal with the disturbance resistance ability of networks. This new concept is obtained from the concentration fluctuation of the sinks. Subsequently, we find the graphical meaning of this concept and prove the sufficient condition of minimum Mixing Potential solution. Then, one graphical approach and its corresponding algorithmic method are proposed in the light of the sufficient condition. Finally, two literature examples are used to illustrate that Mixing Potential could help improving the disturbance

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resistance ability of hydrogen and water networks with minimum utility consumption.

Disturbance Resistance Ability and the Concept of Mixing Potential

In this article, we aim to find a simple and visible concept to measure the disturbance resistance ability of hydrogen networks and water networks. Other than rigorous definition, this concept is based on insights of the disturbance resistance ability and could be used to help improving it. Since the proposed concept is almost identical for both hydrogen and water networks, we do not differentiate these two kinds of networks in the following sections. The differences between these two kinds of networks will be illustrated in the case study.

Let us consider the disturbance resistance ability of a single sink first. The sink is satisfied by several sources. Therefore, any fluctuations in source streams will result in the fluctuation of mixed source stream. We assume the fluctuation comes only from the flow rate of source streams, while the concentration of source streams remains stable. The flow rate fluctuation of source streams will affect both the flow rate and concentration of the mixed source stream. In real process, the flow rate of the mixed source stream can be kept stable by the flow rate control system, while the concentration of the mixed source stream is not controlled. Consequently, we adopt the concentration fluctuation of the mixed source stream to represent the disturbance resistance ability of this satisfying process.

To assess the concentration fluctuation of the mixed source stream, we have to refer to the sources that are used to satisfy the sink. For every sink in the network, there will be at least one source stream to satisfy it. When there is only one source stream to satisfy this sink, the concentration of the sink and the source must be the same. Therefore, the flow rate fluctuation of the source stream will have no influence on the concentration of the mixed source stream, that is, the source stream in this scenario. This is the most operable scenario. However, there are always more than one source streams to satisfy the sink. Let us consider the scenario of two sources satisfying one sink. The material balance of the mixing process can be described as

$$F_1+F_2=F_{\mathrm{D}} \quad (1)$$

$$F_1C_1+F_2C_2=F_{\mathrm{D}}C_{\mathrm{D}} \quad (2)$$

where F_1 and F_2 denote the flow rate of the two sources to the sink, C_1 and C_2 are the concentration of the two sources. F_{D} and C_{D} represent the flow rate and concentration of the sink. Assume the sources are arranged in increasing order of concentration: $C_1<C<C_2$. Let ΔF_1 and ΔF_2 denote the fluctuation value of F_1 and F_2, respectively, then the sink concentration fluctuation value ΔC can be represented as

$$\Delta C=\frac{\Delta F_1C_1+\Delta F_2C_2}{F+\Delta F_1+\Delta F_2} \quad (3)$$

Since the flow rate control system maintains the total flow rate stable, the following equation holds

$$\Delta F_1=-\Delta F_2=\Delta F \quad (4)$$

where ΔF stands for the fluctuation value of source streams. Substitute Eq. 4 into Eq. 3, we obtain

$$\Delta C=\frac{\Delta F}{F}(C_2-C_1) \quad (5)$$

Let σ_F and σ_C denote the standard deviation of ΔF and ΔC, respectively. The relation between σ_F and σ_C is similar to that of the relation between ΔF and ΔC in Eq. 5

$$\sigma_C=\frac{\sigma_F}{F}(C_2-C_1) \quad (6)$$

It should be noted that the distribution of σ_F is not independent and it is affected by the flow rate control system. In this article, we assume the deviations of fluctuations are proportional to the flow rates. Since σ_F is related to both F_1 and F_2, we made further assumption that σ_F is proportional to $F_1\times F_2$. Combining this assumption with Eq. 6, it can be concluded that σ_C is proportional to the term $F_1\times F_2\times(C_2-C_1)$. Let $O_{1,2}$ represent this proportional term

$$O_{1,2}=F_1\times F_2\times(C_2-C_1) \quad (7)$$

then we can minimize σ_C by minimizing $O_{1,2}$. That is to say, the less $O_{1,2}$ is, the smaller the concentration fluctuation of the mixed source stream is.

Next, let us consider the scenario of more than two sources satisfying one sink. Suppose a number of n $(n>2)$ source streams are used to satisfy the sink. The flow rate and concentration of the source streams and the sink are denoted by F_{Sour_i}, C_{Sour_i}, and F_{D}, C_{D}, respectively. Assume that the sources are numbered in the order of increasing concentration, that is, $C_{\mathrm{Sour}_i}<C_{\mathrm{Sour}_{i+1}}$. The mass balance of the process can be described as

$$F_{\mathrm{D}}=\sum_{1}^{n}F_{\mathrm{Sour}_i} \quad (8)$$

$$F_{\mathrm{D}}C_{\mathrm{D}}=\sum_{1}^{n}F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i} \quad (9)$$

The multiple source satisfying scenarios are more complex. Instead of direct derivation, we simplify this scenario by decomposing it into a series of two-source-stream mixing scenarios. Therefore, the result achieved from two-source-stream mixing scenario can be used to deal with this problem. If we cumulate $O_{i,j}$ of every two arbitrary source mixtures, then this summation might be used to approximate the result of multiple source stream mixing scenario. The summation O can be written as

$$O=\sum_{i>j}^{n}\sum_{j=1}^{n}O_{i,j}=\sum_{i>j}^{n}\sum_{j=1}^{n}F_{\mathrm{Sour}_i}F_{\mathrm{Sour}_j}(C_{\mathrm{Sour}_i}-C_{\mathrm{Sour}_j}) \quad (10)$$

Minimizing O provides us a way to reduce the concentration fluctuation of the sink. To compare the results between different sinks, we define the proportion of O to F_D^2 C_{D} as Mixing Potential M

$$M=\frac{O}{F_{\mathrm{D}}^2C_{\mathrm{D}}}\frac{\sum_{i>j}^{n}\sum_{j=1}^{n}F_{\mathrm{Sour}_i}F_{\mathrm{Sour}_j}(C_{\mathrm{Sour}_i}-C_{\mathrm{Sour}_j})}{F_{\mathrm{D}}^2C_{\mathrm{D}}} \quad (11)$$

It should be noted that M is not a rigorous but a simplified representation of concentration flucuation in the multiple source scenario. However, it reflects the concentration flucuation of the mixed source stream to certain extent. Therefore, the disturbance resistance ability of single sink could be improved by minimizing M. If we cumulate the M value of

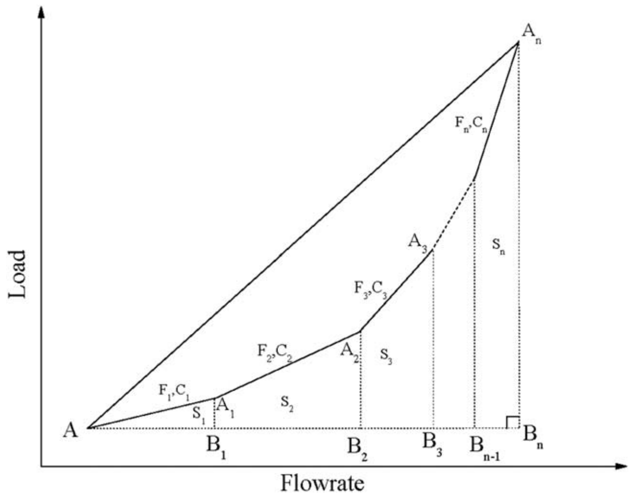

Figure 1. The material balance of mixing scenario with *n* (*n* > 2) sources.

every sink in the network, then we get the Mixing Potential of the whole network. Consequently, the disturbance resistance of the whole network can also be improvd by minimizing Mixing Potential. This new concept provides us a simple way to improve the disturbance resistance ability of the network structure.

The M of the whole network can be minimized by traditional mathematical programming method. However, in this article, we will present simple conceptual method to minimize M for single sinks. Before presenting the method, let us find the graphical meaning of M in the next section.

Graphical Representation of Mixing Potential

The mass balance Eqs. 8 and 9 can also be represented on the flow rate vs. load diagram,[24,25,30] as shown in Figure 1. In this figure, the source streams are represented by lines AA_1, A_1A_2,..., $A_{n-1}A_n$, respectively, while the sink is represented by line AA_n. The source stream lines and the sink stream line form a closed polygon $AA_1A_2...A_n$. The area of polygon $AA_1A_2...A_n$ in Figure 1 can be calculated by the difference between the area of triangle AA_nB_n and the area of polygon $AA_1...A_nB_n$

$$S_{\text{pol}}=S_{\text{total}}-S_{\text{res}} \tag{12}$$

where S_{pol}, S_{total}, and S_{res} represent the area of polygon $AA_1A_2...A_n$, triangle AA_nB_n and polygon $AA_1...A_nB_n$, respectively. The area of right triangle AA_nB_n can be obtained by multiplying the two right-angle sides

$$\begin{aligned}S_{\text{total}}&=\frac{1}{2}(F_1+F_2+\cdots+F_n)(F_1C_1+F_2C_2+\cdots+F_nC_n)\\&=\frac{1}{2}\sum_{i=1}^{n}F_iC_i\sum_{j=1}^{n}F_j\end{aligned} \tag{13}$$

To calculate S_{res}, we decompose polygon $AA_1...A_nB_n$ into a number of n subsections by the dashed lines in Figure 1. The subsections include triangle AA_1B_1 and trapeziums from $A_1B_1B_2A_2$ to $A_{n-1}B_{n-1}B_nA_n$. The area of the subsections are represented by S_1, S_2,..., S_n and the following equation holds

$$S_{\text{res}}=S_1+S_2+\cdots+S_n \tag{14}$$

where S_1, S_2,..., S_n can be calculated by the area formula of triangle and trapezoid as shown in Eq. 15

$$S_1=\frac{1}{2}F_1{}^2C_1 \tag{15-1}$$

$$S_2=\frac{1}{2}(2F_1C_1+F_2C_2)F_2 \tag{15-2}$$

$$S_3=\frac{1}{2}(2F_1C_1+2F_2C_2+F_3C_3)F_3 \tag{15-3}$$

$$\cdots$$

$$S_n=\frac{1}{2}(2F_1C_1+2F_2C_2+\cdots+2F_{n-1}C_{n-1}+F_nC_n)F_n \tag{15-n}$$

Substituting Eqs. 15-1 to 15-n into Eq. 14 and rearranging, we obtain

$$S_{\text{res}}=S_1+S_2+\cdots+S_n=\sum_{i=1}^{n}F_iC_i\sum_{j=i+1}^{n}F_j+\frac{1}{2}\sum_{i=1}^{n}F_i{}^2C_i \tag{16}$$

Substituting Eqs. 13, 16 into Eq. 12 and rearranging

$$\begin{aligned}S_{\text{pol}}&=\frac{1}{2}\sum_{i=1}^{n}F_iC_i\sum_{j=1}^{n}F_j-\sum_{i=1}^{n}F_iC_i\sum_{j=i+1}^{n}F_j-\frac{1}{2}\sum_{i=1}^{n}F_i{}^2C_i\\&=\frac{1}{2}\sum_{i=1}^{n}F_iC_i\left(\sum_{j=1}^{i-1}F_j+F_i+\sum_{j=i+1}^{n}F_j\right)-\sum_{i=1}^{n}F_iC_i\sum_{j=i+1}^{n}F_j\\&-\frac{1}{2}\sum_{i=1}^{n}F_i{}^2C_i=\frac{1}{2}\sum_{i=2,i>j}^{n}\sum_{j=1}^{n}F_iF_j(C_i-C_j)\end{aligned} \tag{17}$$

It should be noted that since $C_i<C_{i+1}$, every term in the right hand side of Eq. 17 is larger than 0. Deviding S_{pol} by S_{total} yields

$$\frac{S_{\text{pol}}}{S_{\text{total}}}=\frac{\sum_{i>j}^{n}\sum_{j=1}^{n}F_iF_j(C_i-C_j)}{FC^2} \tag{18}$$

Substituting Eq. 18 into 9, we have

$$M=\frac{S_{\text{pol}}}{S_{\text{total}}} \tag{19}$$

Equation 19 provides us the graphical meaning of Mixing Potential: M is the area ratio between polygon $AA_1A_2...A_n$ and triangle AB_nA_n. Since S_{total} is constant for one sink, we can minimize M by minimizing S_{pol}. In the next section, we will introduce a sufficient condition for minimizing S_{pol} of a single sink.

Sufficient Condition for Minimizing Mixing Potential

The graphical design method is implemented in the flow rate vs. load diagram. As described in the previous articles,[24,25,30] the source and sink streams can be represented by segments in the flow rate vs. load diagram, respectively. Connecting source/sink segments according to the order of concentration, we can have the source/sink composite curve. In addition, if one sink is satisfied by several sources, the sink and sources can form a closed polygon (or triangle) as shown in Figure 1. Based on the above source composite and the closed polygon, we present the following theorem:

Theorem 1. (Sufficient condition for the minimum M solution)**.** *If a sink is satisfied by a continuous part of the source composite curve, then the area of the achieved closed polygon is the minimum one among all the possible satisfying scenarios.*

Proof. The proof procedure is shown in Figure 2. Figure 2a illustrates a satisfying scenario that meets the condition of Theorem 1. A continuous part of the source composite

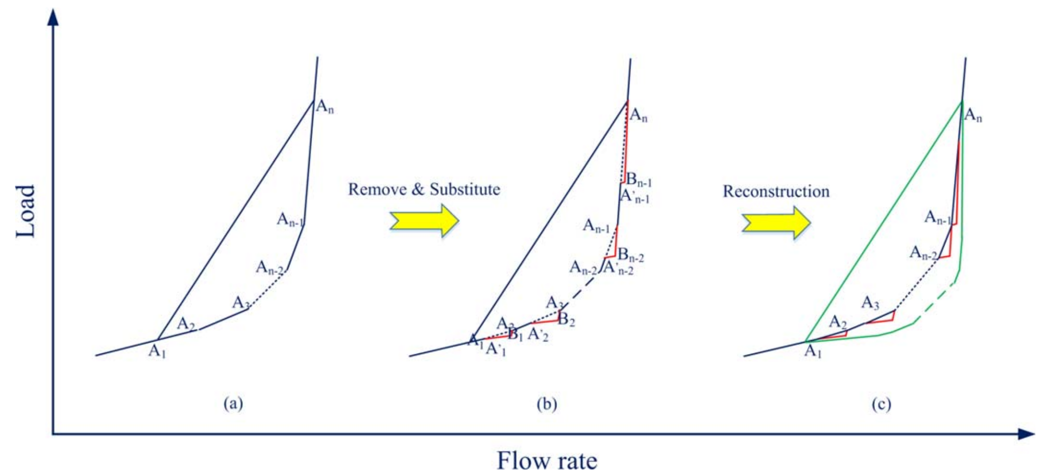

Figure 2. Procedure of proving the condition of Theorem 1.

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

curve, which is represented by segments A_1A_2, A_2A_3,..., $A_{n-1}A_n$ is used to satisfy the sink A_1A_n. In this case, we will prove that the closed polygon $A_1A_2...A_{n-1}A_n$ has the minimum area among the possible satisfying scenarios of sink A_1A_n. We will prove by contradiction: assume certain satisfying scenario constructs smaller closed polygon. This certain scenario can be obtained by shifting the satisfying scenario of Figure 2a. During the shifting procedure, some part of line $A_1A_2...A_{n-1}A_n$ will be removed, while other source streams will be supplemented to replace the removed parts. Without loss of generality, assume the removed parts include part of every segment from A_1A_2 to $A_{n-1}A_n$ which are A'_1A_2, A'_2A_3,..., $A'_{n-1}A_n$ as shown in Figure 2b. According to the definition of source composite curve, source streams between A_1A_2 and $A_{n-1}A_n$ of Figure 2a should have been completely used. Therefore, the concentrations of supplemented source streams are not in the concentration range of A_1A_2 and $A_{n-1}A_n$. Their concentration can be categorized into two classes: either no higher than the concentration of A_1A_2 or no lower than the concentration of $A_{n-1}A_n$. Based on these points, the replaced results is obtained as the red lines shown in Figure 2b. From the figure, it is obvious that the newly formed polygon $A_1A'_1B_1A_2A'_2B_2...A_{n-1}A'_{n-1}B_{n-1}A_n$ is larger than the original one in Figure 2a. If we rearrange the source streams in increasing order of concentration, then a new polygon will be obtained as presented in green lines of Figure 2c, which is larger than the polygons of Figures 2a, b. This contradicts the assumption that certain scenario constructs smaller polygon. The theorem has been proved. It should be noted that Theorem 1 is applicable for a single sink not for entire network involving multiple sinks.

Proposed Design Methods

According to Theorem 1, the minimum M of a single sink can be achieved using part of the source composite curve. In the light of this theorem, corresponding conceptual design approaches can be proposed. We will introduce two conceptual methods: the graphical one and the algorithmic one. Both of the methods comply with Theorem 1.

(1) The graphical method

A hydrogen network example is taken to show the design procedure. The source and sink composite curves are represented in Figure 3a. Hydrogen utility is also taken as one source stream and it can be any segment in Figure 3a, which is depended on the concentration of the hydrogen utility. The sink satisfying procedure is as follows:

Step1: Shift sink AB along the first source stream AH until AB intersects the source composite curve at point B′, as shown in Figure 3b. Then the first sink AB is satisfied by the source stream A′H and HB′. After the first sink is matched, the sources and the sink involved in the match will be eliminated from the diagram. It can be seen that part of

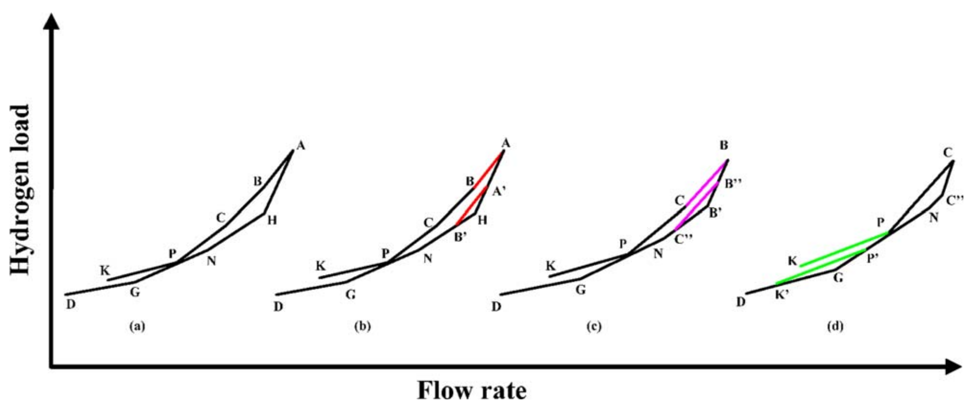

Figure 3. The graphical design procedure.

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

source stream AH, that is, AA′ and part of source stream NH, that is, NB′ are left to satisfy other sinks. The remaining sink and source streams are shown in Figure 3c.

Step2: Shift the next sink BC along BB′ until BC intersects the source composite curve at point C″. Therefore, source streams B″B′, B′C″ are mixed to satisfy the sink BC, as we can see in Figure 3c. Source streams BB″ C″N and NP are remained to match the rest sink CP above the pinch point.

Step3: The sink PK below the pinch point P will also be shifted along the source PG, which is below the pinch point P, until point K intersect the source composite curve at K′. The last sink is satisfied by sources P′G and GK′, as shown in Figure 3d. The remaining streams PP′ and DK′ are the waste.

Note that the sinks are satisfied in the order of decreasing concentration as shown in Figure 3. In fact, this is not a must, and every arbitary order can be adopted to design the network distribution. For example, we can arrange the sinks in the order of singnificance. As a result, the most important sink will minimize its concentration fluctuation first. Also note that a different order might result in a different network distribution.

(2) The algorithemic method

Suppose a hydrogen network with n sources (from Sour_1 to Sour_n) and m sinks (from D_1 to D_m). All of these streams are numbered in the order of increasing hydrogen concentration. The purified product is also included in the n sources. The algorithmic design approach is illustrated in Figure 4 and sink D_j will be taken the as an example to elaborate the four design steps.

Step 1: If there exist a source Sour_i, which has the same concentration as D_j, go to Step 2; else go to Step 3.

Step 2: If $F_{\mathrm{Sour}_i} \geq F_{\mathrm{D}_j}$ which means that the flow rate is enough for sink D_j, then update $F_{\mathrm{sour}_i}=F_{\mathrm{sour}_i}-F_{\mathrm{D}_j}$ and $j=j+1$, and go to Step 1. Else, update $F_{\mathrm{sour}_i}=0$ and $F_{\mathrm{D}_j}=F_{\mathrm{D}_j}-F_{\mathrm{Sour}_i}$. Then go to Step 1.

Step3: As described above, both the flow rate and pure hydrogen load of mixed source stream should not be smaller than the sink. Suppose Sour_r to Sour_p $(1 \leq r < p \leq n)$ are needed at least to satisfy the flow rate of sink D_j, which is given as

$$\sum_{r}^{p-1} F_{\mathrm{sour}_i} + F_{\mathrm{sour}'_p} = F_{\mathrm{D}_j} \tag{20}$$

where $F_{\mathrm{sour}'_p}$ means part of the source Sour_p, that is, $0 < F_{\mathrm{sour}'_p} \leq F_{\mathrm{sour}}$. If $\sum_r^p F_{\mathrm{sour}_p} F_{\mathrm{sour}_i} \geq F_{\mathrm{D}_j} C_{\mathrm{D}_j}$, then go to Step 4; else update $r=r+1$ and repeat this step.

Step 4: Since source streams is numbered in the order of increasing hydrogen concentration, Sour_r has the lowest hydrogen concentration and Sour_p has the highest hydrogen concentration. Therefore, Sour_r and Sour_p are taken as variables to adjust the mixed source stream to satisfy sink D_j sharply. This is shown as

$$xF_{\mathrm{Sour}_r} + \sum_{r-1}^{p-1} F_{\mathrm{Sour}_i} + yF_{\mathrm{Sour}_p} = F_{\mathrm{D}_j} \tag{21}$$

$$xF_{\mathrm{Sour}_r} C_{\mathrm{Sour}_r} + \sum_{r+1}^{p-1} F_{\mathrm{Sour}_i} C_{\mathrm{Sour}_i} + yF_{\mathrm{Sour}_p} C_{\mathrm{Sour}_p} = F_{\mathrm{D}_j} C_{D_j} \tag{22}$$

We can get x and y after solving these equations. If x and y are all in the region [0, 1], we have already got the the exact flow rate of each source streams to satisfy sink D_j. Update $F_{\mathrm{Sour}_r} = (1-x) \quad F_{\mathrm{Sour}_r}$, $F_{\mathrm{Sour}_{p+1}} = (1-y) \quad F_{\mathrm{Sour}_{p+1}}$ (source streams between r and $p+1$ have already been totally used up) and return to Step 1 with another j. Else, if y is bigger than 1, update $p=p+1$ and repeat this step. Else update $r=r+1$ and go to Step 3. Stop when all sinks have been satisfied as we have got the network distribution.

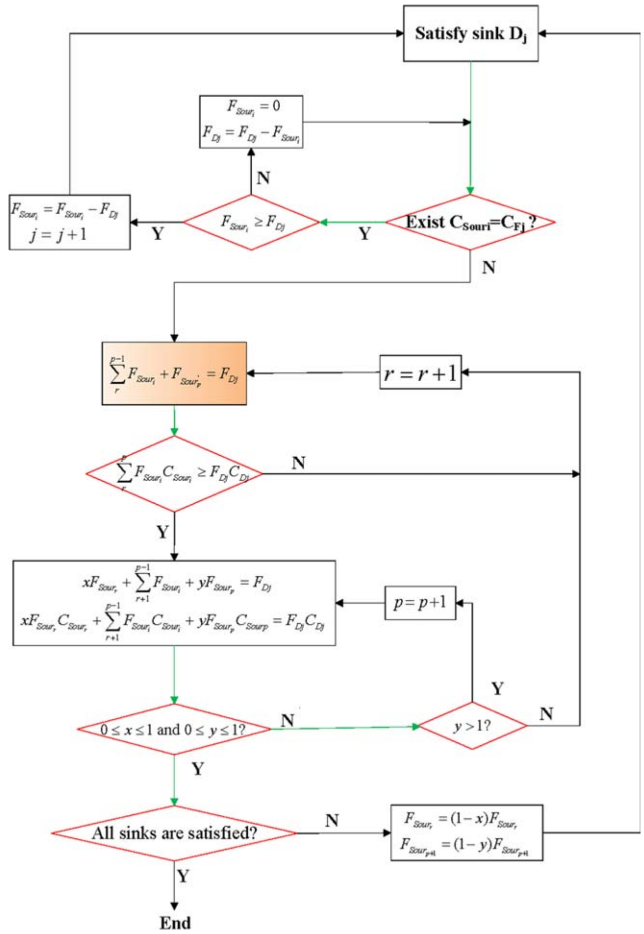

Figure 4. Flow chart for the algorithm design approach.

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

It should be pointed that solving Eqs. 21 and 22 is just like the shifting process described in the graphical approach. Therefore, the graphical method and the algorithemic method correspond to each other.

It should also be noted that the satisfying scenario of Theorem 1 agrees with the principle of the NNA[27,30]: the sink is satisfied by sources whose concentration are closest to the sink. In other words, the sink satisfying scenarios obtained by NNA approach also comply with Theorem 1. Since NNA approach could achieve the minimum utility consumption, the proposed two methods could also achieve the minimum utility consumption. This will be illustrated in the case study.

Case Studies

Example 1—water network design by graphical approach

This example is a water network from Polley and Polley,[34] and we will design this water network using the proposed graphical approach. The detailed process data is shown in Table 1.

Table 1. The Process Data of Example 1

Sink	Flow (t/h)	Concentration (ppm)
1	50	20
2	100	50
3	80	100
4	70	200
1	50	50
2	100	100
3	70	150
4	60	250
Utility	To be determined	0

Step1: Construct the source composite curve with the assumption that the fresh water consumption is 100 t/h (large enough) first, as shown in Figure 5. Then satisfy the sinks through shifting the sink in the contaminant load vs. flow rate diagram.

Step 2: Sinks will be shifted to find the material balance polygon. As described above, sinks that are satisfied in a different order might result in a different network. Sinks satisfied in the order of D_1, D_2, D_3, and D_4 will be taken as an example to be targeted and designed in detail. The first sink D_1, which is represented by AK as shown in Figure 6a, will

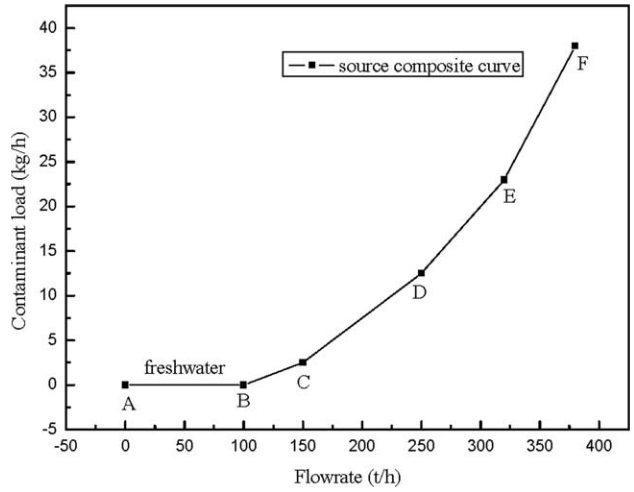

Figure 5. Source composite curve of Example 1.

be shifted along the source composite curve until the end-point K intersects the source composite curve at point K′. The closed triangle A′BK′, which represents the material balance of the sink and sources, is formed. Source streams A′B (fresh water) and BK′ are used to satisfy the sink D_1. Once

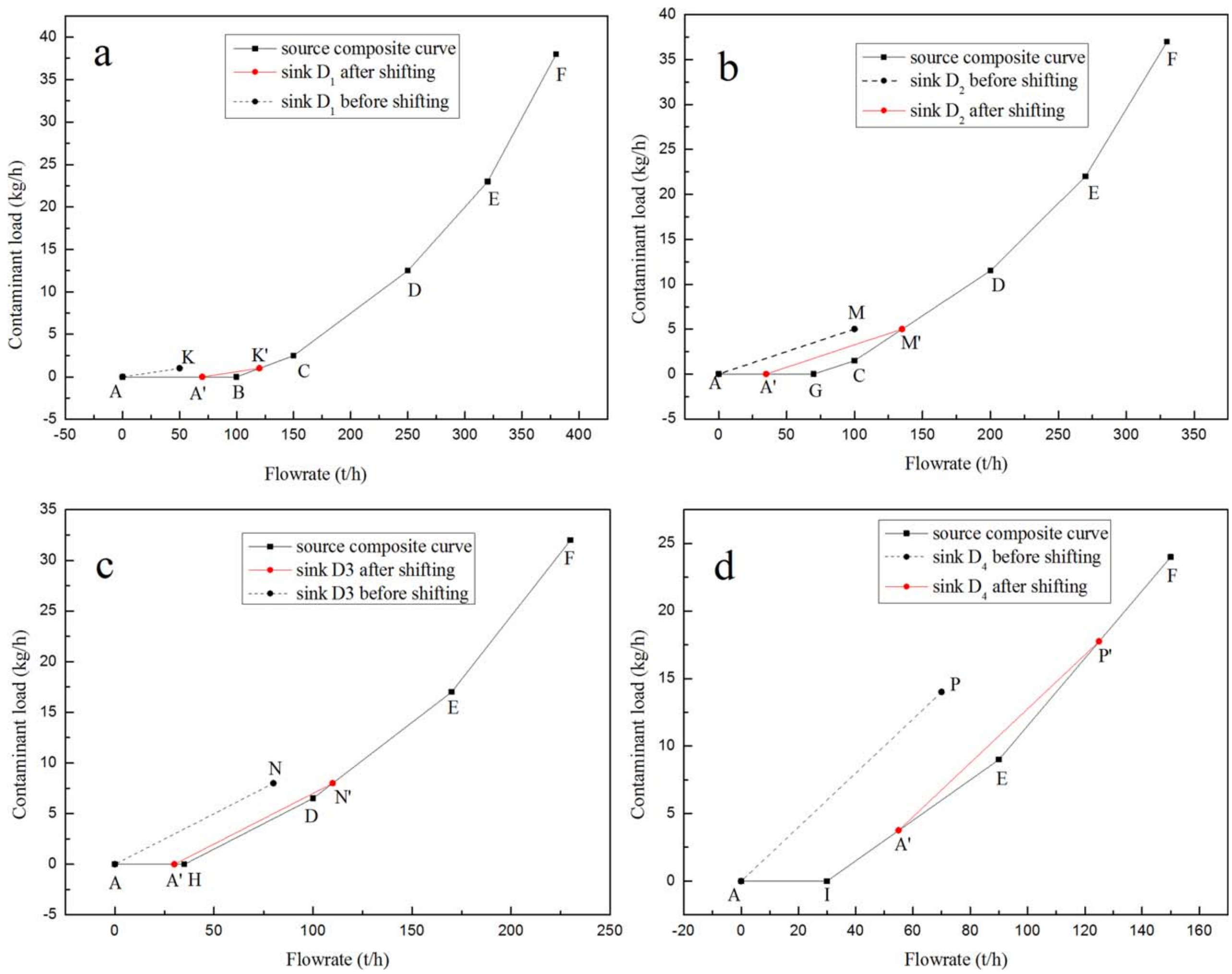

Figure 6. The targeting and design process for Example 1.

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

the sink and sources are matched, they will be eliminated from the diagram. The left source composite curve is shown in Figure 6b, and then the second sink D_2, which is represented by AM, will also be shifted from the origin A along the source segments until point M intersects the composite curve at point M′, as shown in Figure 6b. Thus sink D_2 is satisfied by source streams A′G (fresh water), GC, and CM′. The remaining sources are shown in Figure 6c. The third sink D_3 and the last sink D_4 can be satisfied with the same procedures, which are shown in Figures 6c, d.

We can find that source streams AI, IA′, and P′F are left when all sinks are satisfied, as shown in Figure 6d. Since AI is the fresh water and the projection of AB on X coordinate is 30 t/h, it can be obtained that the minimum fresh water consumption is 70 t/h, which is the same result achieved by Polley and Polley[34] and Agrawal and Shenoy[27]. Source streams IA′ and P′F are the waste. The network is shown in Figure 7a.

A number of water network structures can be achieved via different sink satisfying orders. In this case, we can see that the last sink D_4 can only be satisfied by two sources with the highest contaminant concentration, which are DE and EF in Figure 5. Therefore, it will not affect the network configuration whether it is satisfied in the front or rear order. When the designing orders are: D_1, D_2, D_3; D_2, D_1, D_3; D_2, D_3, D_1; D_3, D_1, D_2; and D_3, D_2, D_1, respectively, other five network configurations can be achieved. The obtained network structures are shown in Figures 7a, b, c, d, e, respectively. It should be noted that the order of D_3, D_1, D_2 and D_1, D_3, D_2 will get the same network.

Then we will choose the most operable network with the proposed approach. The Mixing Potential of each sink is shown in Figure 8. From the results, it is easy to see that the same sink in different network configurations may be satisfied by different source streams and these different mixing scenarios have different Mixing Potentials. Taking sink D_1 as an example, three different mixing scenarios can be used to satisfy sink D_1, among which the mixing scenario to satisfy sink D_1 in Networks 1 and 4 are the most operable. The total Mixing Potentials of all sinks in one network configuration can be used to compare the disturbance resistance ability of the network. We can find that Network 4 has the minimum Mixing Potential among the five networks configurations, which means that Network 4 is more operable according to the theory we have proposed above.

Example 2—hydrogen network design by algorithmic approach

This example is taken from Alves and Towler.[21] The system consists of four hydrogen consuming processes: hydrogen cracker unit (HCU), naphtha hydrotreater (NHT), cracked naphtha hydrotreater (CNHT), and a diesel hydrotreater (DHT). The feed of these units can be considered as hydrogen demands while the outlet streams can be taken as sources. There are also two individual hydrogen sources: the catalytic reforming unit (CRU) and the steam reforming unit (SRU). Besides, the hydrogen utility with the concentration of 95 mol % is also available in this system. The detailed process data is shown in Table 2.

This example has been studied by many researchers with or without purification unit. Since most refineries use purification unit to reduce the hydrogen utility consumption, we will use the results targeted by pinch sliding approach[35] to design hydrogen networks with purification units. The minimum hydrogen utility consumption is 196.77 mol/s and the purified product 64.33 mol/s with 98% hydrogen concentration. These hydrogen source streams are numbered in the order of increasing hydrogen concentration, therefore, the purified product is taken as source stream $Sour_8$. The hydrogen sinks are numbered in the order of decreasing concentration. The inlet of the purifier is 94.8 mol/s with hydrogen concentration 70%, that is, to say the purifier will also be taken as a special sink, which can be satisfied only by $Sour_1$. We will satisfy sinks in the order of decreasing hydrogen concentration and sink D_1 is taken as an example to show the detailed design process.

Step 1: Since no source stream has the same concentration as D_1, then go to Step 3 directly.

Step 3: Source streams with lower hydrogen concentration will be given priority to satisfy the sink. Therefore, source streams $Sour_1$, $Sour_2$, and $Sour_3$ will be used first to satisfy the flow rate demand of sink D_1, which is shown as

$$F_{\mathrm{Sour}_1}+F_{\mathrm{Sour}_2}+F'_{\mathrm{Sour}_3}=457.4+346.5+1691.1=F_{\mathrm{D}_1} \quad (23)$$

Then compare $\sum_1^3 F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i}$ and $F_{\mathrm{D}_1}C_{\mathrm{D}_1}$, which are given as

$$\sum_1^3 F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i}=457.4\times 0.7+346.5\times 0.73 +1801.9\times 0.75=1924.55 \quad (24)$$

$$F_{\mathrm{D}_1}C_{\mathrm{D}_1}=2495\times 0.8061=2011.22 \quad (25)$$

Since $\sum_1^3 F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i} < F_{\mathrm{D}_1}C_{\mathrm{D}_1}$, update $r=2$ and repeat this step. Source stream $Sour_2$, $Sour_3$, $Sour_4$, and $Sour_5$ will be used to satisfy sink D_1

$$F_{\mathrm{Sour}_2}+F_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}+\mathrm{F}'_{\mathrm{Sour}_5}=346.5+1801.9 +138.6+208=F_{\mathrm{D}_1} \quad (26)$$

Then compare $\sum_2^5 F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i}$ and $F_{\mathrm{D}_1}C_{\mathrm{D}_1}$, which is given as

$$\sum_2^5 F_{\mathrm{Sour}_i}C_{\mathrm{Sour}_i}=346.5\times 0.73+1801.9\times 0.75+138.6\times 0.75 +415.8\times 0.8=2040.96 > F_{\mathrm{D}_1}C_{\mathrm{D}_1} \quad (27)$$

Therefore, go to Step 4.

Step 4: Solve the equations to get the exact flow rate of each source. Source stream $Sour_2$, $Sour_3$, $Sour_4$, and $Sour_5$ will be taken into consideration first

$$xF_{\mathrm{Sour}_2}+F_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}+yF_{\mathrm{Sour}_5}=F_{\mathrm{D}_1} \quad (28)$$

$$xF_{\mathrm{Sour}_2}C_{\mathrm{Sour}_2}+F_{\mathrm{Sour}_3}C_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}C_{\mathrm{Sour}_4}+yF_{\mathrm{Sour}_5}C_{\mathrm{Sour}_5}=F_{\mathrm{D}_1}C_{\mathrm{D}_1} \quad (29)$$

The results are: $x=-4.6277$, $y=5.19$. Since x and y are not in the regin [0, 1] and $y>1$, update $p=6$ and solve the following Eqs. 30 and 31

$$xF_{\mathrm{Sour}_2}+F_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}+F_{\mathrm{Sour}_5}+yF_{\mathrm{Sour}_6}=F_{\mathrm{D}_1} \quad (30)$$

$$xF_{\mathrm{Sour}_2}C_{\mathrm{Sour}_2}+F_{\mathrm{Sour}_3}C_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}C_{\mathrm{Sour}_4} +F_{\mathrm{Sour}_5}C_{\mathrm{Sour}_5}+yF_{\mathrm{Sour}_6}C_{\mathrm{Sour}_6}=F_{\mathrm{D}_1}C_{\mathrm{D}_1} \quad (31)$$

The results are: $x=-1.3595$, $y=0.9775$. Since x is not in the region [0, 1] and $y<1$, update $r=3$ and return to Step 3.

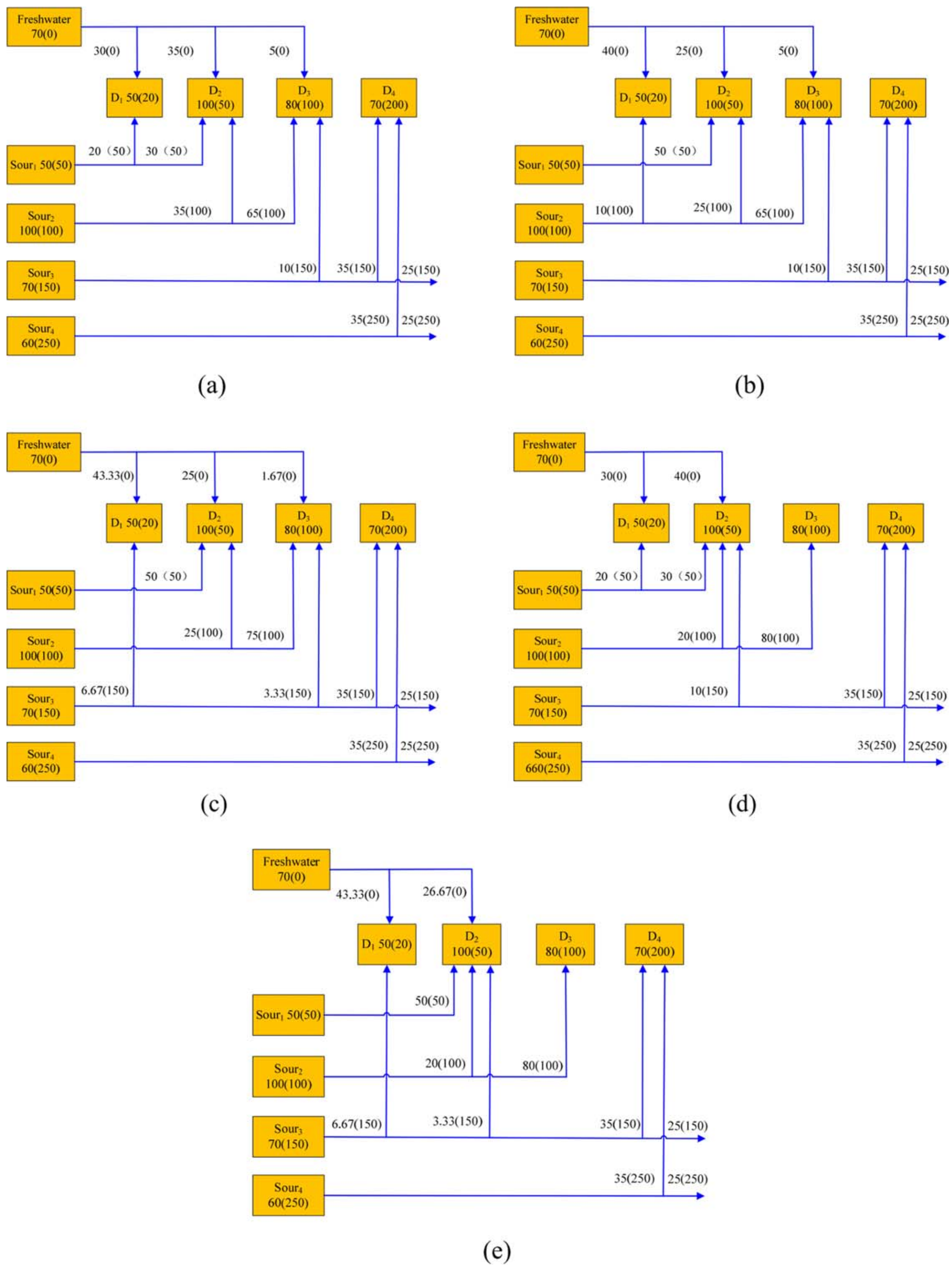

Figure 7. The achieved water networks for Example 1.

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

Step 3: Source stream Sour_3, Sour_4, Sour_5, and Sour_6 are used to satisfy sink D_1

$$F_{\text{Sour}_3}+F_{\text{Sour}_4}+F_{\text{Sour}_5}+F'_{\text{Sour}_6}=1801.9+138.6+415.8+138.7=F_{D_1} \tag{32}$$

$$\begin{aligned}F_{\text{Sour}_3}C_{\text{Sour}_3}+F_{\text{Sour}_4}C_{\text{Sour}_4}+F_{\text{Sour}_5}C_{\text{Sour}_5}+F_{\text{Sour}_6}C_{\text{Sour}_6}\\ =1801.9\times0.75+138.6\times0.75+415.8\times0.8\\ +623.8\times0.93=2368.149\end{aligned} \tag{33}$$

Since $\sum_3^6 F_{\text{Sour}_i}C_{\text{Sour}_i} > F_{D_1}C_{D_1}$, then go to Step 4.

Step 4: The equations are given as

$$xF_{\text{Sour}_3}+F_{\text{Sour}_4}+F_{\text{Sour}_5}+yF_{\text{Sour}_6}=F_{D_1} \tag{34}$$

$$xF_{\text{Sour}_3}C_{\text{Sour}_3}+F_{\text{Sour}_4}C_{\text{Sour}_4}+F_{\text{Sour}_5}C_{\text{Sour}_5}+yF_{\text{Sour}_6}C_{\text{Sour}_6}=F_{D_1}C_{D_1} \tag{35}$$

We can find that x is 0.7095 and y is 1.0614. Since y is bigger than 1, update $p=7$. Therefore, Eqs. 34 and 35 turn into

$$xF_{\text{Sour}_3}+F_{\text{Sour}_4}+F_{\text{Sour}_5}+F_{\text{Sour}_6}+yF_{\text{Sour}_7}=F_{D_1} \tag{36}$$

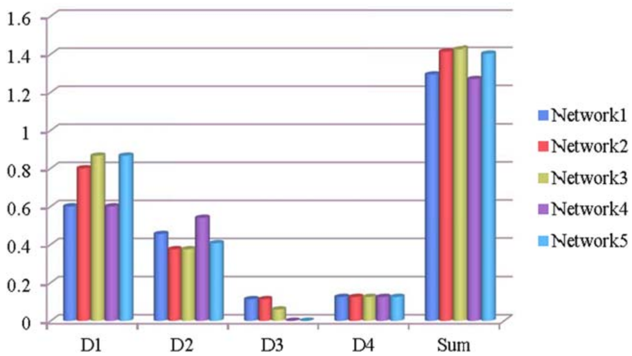

Figure 8. The Mixing Potential of different water networks for Example 1.

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

Table 2. Process Data of Example 2

No.	Sinks	Flow (mol/s)	Hydrogen concentration (mol %)
D1	HCU	2495.0	80.61
D2	NHT	180.2	78.85
D3	DHT	554.4	77.57
D4	CNHT	720.7	75.14
Sour1	CNHT	457.4	70.00
Sour2	DHT	346.5	73.00
Sour3	HCU	1801.9	75.00
Sour4	NHT	138.6	75.00
Sour5	CRU	415.8	80.00
Sour6	SRU	623.8	93.00
Sour7	Utility	To be determined	95.00

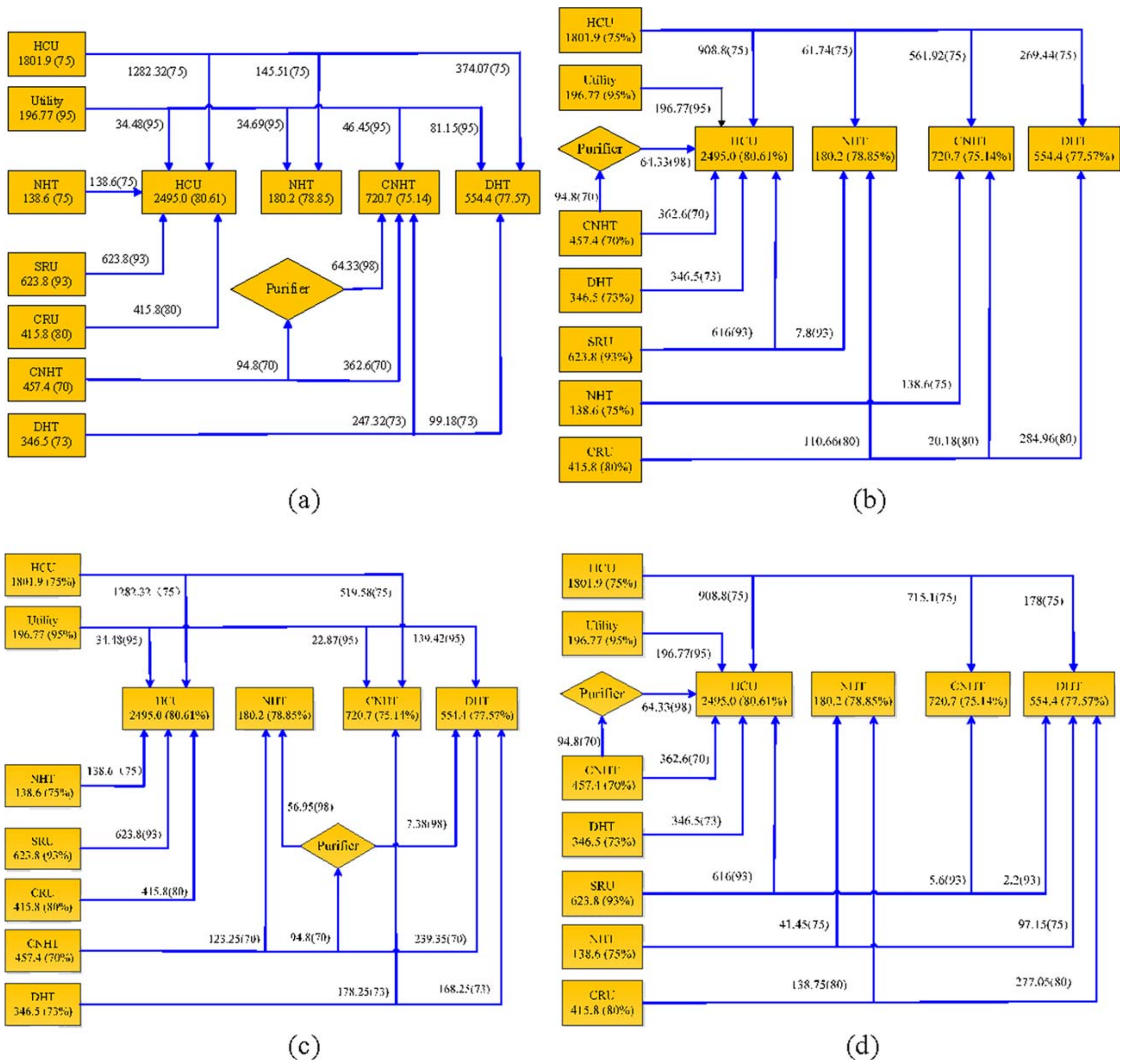

Figure 9. The achieved hydrogen networks for Example 2.

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

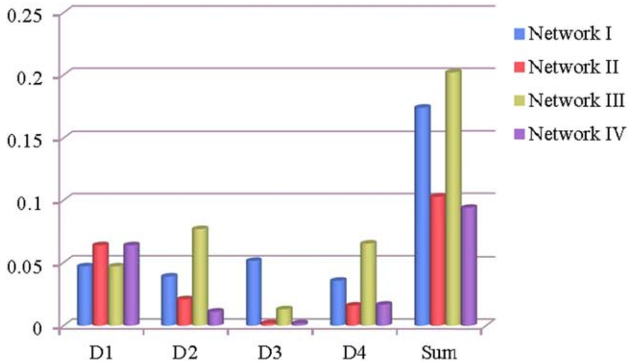

Figure 10. The Mixing Potential of different hydrogen networks for Example 2.

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

$$xF_{\mathrm{Sour}_3}C_{\mathrm{Sour}_3}+F_{\mathrm{Sour}_4}C_{\mathrm{Sour}_4}+F_{\mathrm{Sour}_5}C_{\mathrm{Sour}_5}+F_{\mathrm{Sour}_6}C_{\mathrm{Sour}_6}+yF_{\mathrm{Sour}_7}C_{\mathrm{Sour}_7}=F_{\mathrm{D}_1}C_{\mathrm{D}_1} \quad (37)$$

We can find that x is 0.7117 and y is 0.1752 after solving the equations. Therefore, the flow rate of Sour_3 and Sour_7 that are used to satisfy sink D_1 are 1282.32 and 34.48 mol/s, respectively.

Sink D_1 is satisfied after the proposed procedures above. Then update $\mathrm{Sour}_3 = 519.58$ mol/s, $\mathrm{Sour}_7 = 62.29$ mol/s, and $\mathrm{Sour}_4 = \mathrm{Sour}_5 = \mathrm{Sour}_6 = 0$. Other sinks can also be satisfied with the same procedures. When all the sinks are satisfied, we will get the network distribution. It should be noted that, in this case, source streams Sour_3 and Sour_4 have the same hydrogen concentration and the network distribution may be different when the number of these two steams change. The hydrogen network distribution, in this case, is shown in Figure 9a.

The sinks can also be satisfied in the order of increasing hydrogen concentration, that is, D_4, D_3, D_2, and D_1. The hydrogen network as shown in Figure 9b can also be obtained with the same design procedure. When the sinks are satisfied in the order of decreasing flow rate, that is, D_1, D_4, D_3, and D_2, the network configuration as shown in Figure 9c can be achieved. When the sinks are satisfied in the order of increasing flow rate, that is, D_2, D_3, D_4, and D_1, the network distribution is shown in Figure 9d.

More streams mean more network configurations. The four network configurations are obtained according to the order of sink concentration and flow rate as described above. These networks can also be distinguished by Mixing Potential. The results are shown in Figure 10. It is easy to see that network IV has the minimum Mixing Potential among these achieved networks. Therefore, according to the theory, we proposed above, Network 4 is more operable among these four networks.

Conclusion

Mixing Potential concept has been proposed in the present work to reflect the disturbance reistance ability of hydrogen and water networks. This concept is derived from measuring the concentration fluctuation of a single sink. Although simplifications have been made in the derivation process, minimizing Mixing Potential could improve the disturbance resistance ability of networks significantly. In addition, this concept is visible in the load vs. flow rate diagram: it can be represented by the area of polygons, which is formed by the sink and the source streams, which are used to satisfy the sink.

A sufficient condition for minimizing Mixing Potential has been proved. Based on this condition, a graphical design method and its corresponding algorithmic method are proposed to design hydrogen and water networks with minimum utility consumption. The sinks are satisfied in different orders for both methods. Different satisfying orders might result in different values of Mixing Potential for both a single sink and a whole network. The disturbance resistance ability of one sink could be improved by giving priority order to be satisfied. The network structure with higher disturbance resistance ability can be identified by comparing the total Mixing Potentials of the obtained networks. The design processes of two literature examples of water network and hydrogen network show the effectiveness of graphical method and algorithmic method, respectively. In the future research, we will focus on the comparison of Mixing Potential with the actual fluctuation and the assessment of the accuracy of the simplified expression.

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Notation

F = flow rate
C = concentration
σ = standard deviation
Sour = source stream
D = sink
M = Mixing Potential
S = area
F_{Sour_i} = the flow rate of source stream i
F_{Sour_p} = the flow rate of source stream p
C_{Sour_i} = the concentration source stream i
C_{Sour_p} = the concentration source stream p
F_{D_j} = the flow rate of sink j
C_{D_j} = the concentration of sink j
S_{total} = the total area of triangle
S_{res} = the area of the rest part
S_{pol} = the area of polygon

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