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Judicious generation of alternative water network designs with manual evolution strategy

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ABSTRACT

This study is aimed to judiciously generate the desired alternative configurations of a given single-contaminant water-using system under the constraints of minimum freshwater usage, minimum match number and minimum total throughput. A generalized source-shift procedure is proposed for this purpose, which can be applied manually by evolution from a preliminary network which requires minimum freshwater usage. Systematic implementation guidelines are also provided to perform the evolution steps. In addition, the minimum interconnection number can be estimated in advance and the total number of promising alternative solutions can also be determined *a priori*. Six examples are presented in this paper to demonstrate the effectiveness and benefits of applying our method.

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1. Introduction

Industrial water network synthesis (Jezowski, 2010; Mann and Liu, 1999) has been an active research area in process systems engineering for more than a decade. The available design methods can be classified into two general types, i.e., the pinch based and the mathematical programming based approaches. A full review on the former approach is given by Foo (2009), while Faria and Bagajewicz (2010a) presented a thorough survey of the latter.

To take into account of the recent shift in setting priority among conflicting criteria for water network design, it becomes necessary to place emphasis on water conservation from the outset and then address other critical issues, e.g., capital cost, safety and operability, etc., at later stages. For any water-using process, it is usually possible to identify more than one network structure that features minimum freshwater usage, minimum match number and minimum total throughput simultaneously. In order to select the most appropriate design, these initial candidates should obviously be identified as many as possible in cases when some of the "promising" solutions may have infeasible layouts or are difficult to be implemented in reality. Two distinct approaches have been taken to accomplish this task after a preliminary network configuration is obtained. One is to partially or totally redesign the network, while the other is basically evolutionary in nature. In the former case, two distinct strategies have been proposed:

- If the pinch-based design procedure (Dunn and Wenzel, 2001; Prakash and Shenoy, 2005a; Savelski and Bagajewicz, 2001; Wang and Smith, 1994) is adopted to synthesize a preliminary optimal network, it was suggested to go back to an intermediate step and consider the other branch options.
- If the mathematical programming method is used for generating the basic optimal solution, the common practice is to rerun the same model with
 - a different initial guess and/or an alternative solver (Bagajewicz and Savelski, 2001; Li and Chang, 2007),
 - additional cutting conditions (Ahmetovic and Grossmann, 2011; Faria and Bagajewicz, 2010b; Poplewski et al., 2010), or
 - the "solution pool" technique (Li and Chang, 2011b).

In practical applications, it is usually time consuming to implement the pinch-based procedure for the purpose

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Nomen	clature
Δf	the reduced flowrate
ΔM	mass load
ci	inlet concentration
CO	outlet concentration
f	flow rate
K	total number of source shift sets
N, n	total number
SR	water source
Supersc	ripts
lim	limit
W	freshwater
тах	maximum
in	inlet
out	outlet
Subscri	ots
2s	two-source shift
cf	configuration
i	independent source-shift set
LP	loop
S	source
ST	subset
3s	three-source shift
D	demand
j	decoupled candidate shift
М	match
S	shift
u, u′	water-using unit

of generating multiple configurations. In addition, since the mathematical programming method is essentially a blackrectangle approach, only the final designs can be obtained and some of the potentially useful insights which could be gained in the solution process are often ignored entirely (Das et al., 2009).

On the other hand, since the evolutionary approach is implemented via modifying a base-case solution (Ng and Foo, 2006; Prakash and Shenoy, 2005b), it is in general simpler and therefore more appealing than the aforementioned pinchbased method if a preliminary network configuration can be made available. Prakash and Shenoy (2005b) first proposed a so-called source-shift algorithm (SSA) to evolve from a preliminary design to network structures with fewer matches. Ng and Foo (2006) later argued that the original version of sourceshift strategy was iterative which could only be applied in a trial-and-error fashion. Two heuristic rules were therefore introduced in the improved source-shift algorithm (ISSA) to circumvent this drawback. The idea of water path, which is similar to the well-established concept of heat load path in HEN design (Linnhoff and Hindmarsh, 1983), was also proposed to relax the upper bound of freshwater consumption rate so as to simplify network configuration. Recently, Das et al. (2009) proposed four additional evolution techniques according to the concepts of loop breaking and path relaxation for the purpose of deriving simple designs from a preliminary resource allocation network (RAN). Although successful applications were reported, the total number of alternative configurations was not targeted and resource penalty can not always be avoided during the evolution procedure.

It should be pointed out that the available evolution methods were mainly developed for the fixed-flowrate operations (Polley and Polley, 2000). The inlet and outlet streams of every fixed-load operation in the previous applications were treated as independent demand and source, while the material-balance relation between their flow rates was totally neglected (Das et al., 2009; Prakash and Shenoy, 2005b; Ng and Foo, 2006). Examples of the former operations could include the boilers, cooling towers and reactors in which water does not play the role of a mass separating agent (MSA). The water flow rates at the inlet and outlet of such unit are fixed, but may not necessarily be equal. Examples of the latter operations include washing, scrubbing and extraction, etc., in which water is used as the only MSA. The inlet and outlet water flow rates of every fixed-load operation are equal if water loss or gain is not considered, and these values are allowed to vary as long as the given load is removed (Prakash and Shenoy, 2005a). Notice also that there are virtually no systematic guidelines available to perform the source-shift steps and, furthermore, there is no guarantee that all promising solutions of the same quality can be obtained even for a small problem.

To improve the current evolution practice, it is our intention to develop a generalized source-shift procedure and the corresponding implementation guidelines which can be applied to any single-contaminant water-using network with fixedflowrate and/or fixed-load units. The goal of evolution in the present study is to obtain the desired alternative solutions with minimum freshwater usage, minimum number of interconnections and minimum total throughput. It should be noted that, although the available mathematical programming methods can also be used to obtain all promising water networks (Li and Chang, 2011b), the proposed manual evolution method is still useful due to the need to judicious generated the most satisfied one according to other less tangible criteria, e.g., safety in realistic designs. In addition, it is possible to obtain two important design targets to facilitate efficient application of the evolution procedure:

- 1. The minimum number of interconnections in a water network can be calculated a priori according to Euler theorem (Prakash and Shenoy, 2005b).
- The total number of promising alternative networks can be determined in advance without generating all alternative configurations.

Since the existence of alternative configurations can only be attributed to source shifts, *all* possible promising solutions can always be found with the proposed evolution procedure. This useful insight obviously cannot be incorporated in a mathematical programming model. Finally, it should be pointed out that, although the proposed evolution procedure is designed mainly for the single-contaminant systems, it can be extended for multi-contaminant applications as well. The interested readers can refer to Li and Chang (2011a) for further details.

This paper is structured as follows. A problem statement is first provided in the next section. The guidelines and systematic implementation procedures for performing the generalized source-shift operations are then presented in Section 3. This method is next illustrated with a series of examples designed to demonstrate its applicability in a wide spectrum of different problems. Specific conclusions are given at the end of this paper.

2. Problem statement

Given a minimum-consumption water-using network (Li and Chang, 2007; Prakash and Shenoy, 2005a; Savelski and Bagajewicz, 2001; Wang and Smith, 1994) in which the outlet concentration of every fixed-load unit reaches its upper bound (Savelski and Bagajewicz, 2000), the objective of present synthesis task is to systematically evolve from this given design to generate the desired alternative solutions with the minimum freshwater consumption rate, the minimum number of interconnections and the minimum total throughput.

Specifically, the following process data are assumed to be available: (1) the mass load and the upper bounds of inlet and outlet concentrations of each fixed-load unit; (2) the required supply rate and contaminant concentration of each internal source (or output from each fixed-flowrate unit); (3) the required water flow rate and the maximum allowable concentration of each internal demand (or input to each fixedflowrate unit); (4) the contaminant concentration of every external source (or freshwater stream); (5) the upper limit of contaminant concentration of every external demand (or effluent stream). The evolution results should obviously be the desired alternative network designs. The design specifications of each network should include: (1) the interconnections and their flow rates and concentrations, and (2) the throughput of each unit and its inlet concentration.

3. Available methods

The primary purpose of SSA (Prakash and Shenoy, 2005b) is to identify different network configurations on the basis of a given set of design criteria. This objective can be achieved manually with *source shift*, i.e., moving a water source from one sink to another without violating the requirements on the flow rates and contaminant concentrations at the sinks. This evolutionary operation is accomplished by mixing two or three different sources to fulfill the sink requirements. Usually, the goal of such a shift is either (1) to eliminate one or more interconnections in the preliminary network in order to yield a less complex structure or (2) to generate an alternative network configuration when the total match number is already at its minimum value (Prakash and Shenoy, 2005b).

Since there were no systematic guidelines, the implementation procedure of SSA could be very tedious and cumbersome (Ng and Foo, 2006). The following two criteria were therefore introduced in ISSA to identify suitable candidates for source shifts:

- The sink and source concentrations must be the same.
- The water flow rate available at the source should be higher than, or equal to, that required by the sink.

It should be noted that even ISSA cannot be used to systematically identify all source-shift candidates which can lead to a simpler structure. To illustrate this point, let us consider the *matching matrix* (Prakash and Shenoy, 2005b) in Fig. 1. The rows and columns of this matrix are associated with sources (S0–S3) and sinks (D1 and D2), respectively, while their process data are given in the cells in the far-left column and in the top row. In each cell, the concentration in ppm and the water flow rate in t/h are provided within and outside of the brace, respectively. For illustration convenience, a match (or

F t/hr {C ppm}	Streams	D1 40{50}		D2 100{150}
$20\{0\}$ $20\{100\}$ $50\{100\}$ $50\{200\}$	S0 S1 S2 S3	20 20	$\stackrel{20}{\xrightarrow{20}}$	20 30 50

Fig. 1 - Matching matrix for a motivation example.

matches) between a sink SK and its source(s) is represented in this paper as

$$[f_1 SR_1 + f_2 SR_2 + f_3 SR_3 + \cdots]_{SK}$$
(1)

where SR_i (i = 1, 2, ...) denotes the ith water source and f_i represents the flow rate of the corresponding match. These match water flow rates are specified in the corresponding cells in the matching matrix. It should be made clear that there are really no source-shift opportunities if SSA or ISSA is applied to the example considered here. However, one match in the original design can nonetheless be eliminated if the sources of matches [20S1]_{D2} and [20S2]_{D1} are interchanged as indicated in Fig. 1, in which the shift direction is indicated with an arrow and the shifted flow rate is specified just above the arrow. Basically the same notations will be followed in the subsequent figures and tables. The resulting design is shown in Fig. 2. Notice that the concentrations of S1 and S2 in this scenario are identical and such a two-source shift is excluded in either SSA or ISSA.

4. Match constraints for fixed-load operations

As mentioned earlier, both SSA and ISSA can be used for generating network designs with fixed-flowrate units only. It is therefore necessary to extend the available source-shift methods to the fixed-load operations. Let us assume that that there is no water loss or gain and thus the flow rates of water entering and leaving any such unit should be identical. Following is a widely accepted unit model (Wang and Smith, 1994):

$$\Delta M = f(co - ci) \tag{2}$$

where ΔM is a constant model parameter representing the mass load; f is the throughput; co and ci are the process variables denoting the inlet and outlet contaminant

F t/hr{C ppm}	Streams	D1 40{50}	D2 100{150}
$20\{0\}$ $20\{100\}$ $50\{100\}$ $50\{200\}$	S0 S1 S2 S3	20 20	50 50

Fig. 2 – Matching matrix after two-source shift for the motivation example.



Fig. 3 - A typical water using unit.

concentrations, respectively. In addition, the inlet and outlet concentrations must not exceed the specified upper limits, i.e.,

$$ci \le Ci^{max}$$
 $co \le Co^{max}$ (3)

Savelski and Bagajewicz (2000) showed that, if the total freshwater consumption rate of a water network is kept at the minimum level, it is always possible to create a design in which the outlet concentration of every fixed-load unit reaches the upper bound. Although there can also be other network configurations that meet the same freshwater targets, the corresponding solutions have larger throughput and thus call for larger unit sizes and higher costs. On the other hand, Eq. (2) suggests that the throughput may be reduced by lowering the inlet concentration. Therefore, it is clear that a fixed-load unit should not accept the self-recycle stream or any reuse stream if its contaminant concentration is equal to (or even greater than) the maximum allowable outlet concentration. Such self-recycle and/or reuse streams at the inlet of a fixed-load unit are referred to as the futile streams in the minimum-consumption network, while the remaining streams are called the valid streams. Notice that a futile stream increases the inlet concentration and also throughput, but contributes nothing to remove the mass load. While keeping the concentrations and flow rates of all valid streams unchanged, the total throughput of a minimum-consumption water network can be reduced to the lowest possible level simply by deleting all the futile streams. It is obvious that the self-recycle streams can be deleted directly. On the other hand, the deletion of a futile reuse stream can be accomplished by rerouting it to bypass the corresponding fixed-load unit. This throughput reduction approach can be justified with the following theorem:

Theorem (Stream deletion conditions). Given a minimumconsumption single-contaminant water network in which the outlet concentration of every fixed-load unit reaches the upper limit, its total throughput can be minimized by removing all futile streams under the condition that the flow rates and concentrations of all valid streams remain unchanged.

Proof. To fix idea, let us consider the typical fixed-load unit shown in Fig. 3. Let us assume that its outlet concentration reaches the maximum allowable level (Co_u^{max}) and both freshwater (whose flow rate is f^W and contaminant concentration is 0) and reuse stream (whose flow rate is $f_{u',u}$ and contaminant concentration is $co_{u'}$) are consumed by this unit. According to the necessary conditions of concentration monotonicity (Savelski and Bagajewicz, 2000), it can be deduced that $co_{u'} \leq Co_u^{max}$.

It is clear that f^W cannot be decreased since it is the flow rate of a valid stream. Thus, the throughput of this unit can only be reduced by cutting down the flow rate of reuse stream. By establishing contaminant mass balance before and after throughput reduction, the following results can be obtained according to Eq. (2):

$$f_{u',u}co_{u'} + \Delta M = (f_{u',u} + f^{W})Co_{u}^{max}$$
(4)

$$(f_{u',u} - \Delta f) co_{u'} + \Delta M = (f_{u',u} - \Delta f + f^{W}) Co_{u}^{max}$$
(5)

where Δf denotes the reduced throughput. Further subtracting Eq. (5) from Eq. (4) yields:

$$\Delta f co_{u'} = \Delta f Co_u^{max} \tag{6}$$

This implies that either $co_{uv} = Co_u^{max}$ or $\Delta f = 0$ must be true. Thus, if $\Delta f > 0$, the reduced throughput can only be attributed to the futile stream(s). Furthermore, the overall throughput of the network cannot be reduced anymore if all futile streams are removed.

Finally, the flow rate f defined in Eq. (2) should not be allowed to exceed the limiting flow rate of fixed-load unit (F^{lim}) when implementing the evolution steps, i.e.

$$f \le F^{\lim} \tag{7}$$

where F^{lim} is defined as:

$$F^{lim} = \frac{\Delta M}{(Co^{max} - Ci^{max})}$$
(8)

This heuristic constraint is used as an auxiliary rule in this study to preclude the potentially degenerate configurations and allow designer focusing on the more favorable ones. Finally, notice that a self-recycle can be easily reintroduced when a fixed flow rate of F^{lim} is required (Dunn and Wenzel, 2001; Wang and Smith, 1995).

5. Generalized source-shift procedure

As mentioned previously, there is a definite need to develop a systematic implementation strategy to guide the source-shift operations. To this end, the evolution procedure given in Fig. 4 can be applied to a preliminary network with minimum freshwater usage. A detailed description of each step is provided below:

- Step 0: Delete the futile stream(s) at the inlet of each fixed-load unit. And certainly, this step should be skipped if there is no futile streams in the preliminary network.Step 1: Target the minimum match number.
 - As pointed out by Prakash and Shenoy (2005b), any water network can be characterized by a bipartite graph with nodes denoting water streams (sources and demands) and edges denoting matches. The number of matches (N_M) can then be calculated according to Euler's network theorem:

$$N_M = N_S + N_D + N_{LP} - N_{ST}$$
⁽⁹⁾

where N_S and N_D represent the numbers of water sources (including both internal and external sources) and demands (including both internal and external sinks or demands), respectively; N_{LP} is the number of *independent* loops; N_{ST} is the number of *indepen*dent subsets. A loop in the water network can be



Fig. 4 - Generalized evolution procedure for water-using network.

conveniently identified on the matching matrix by starting at a match and returning to the same match via a set of horizontal and vertical paths through nonzero entries. An independent subset is a set of sources and demands which can be perfectly matched and constitute an independent subproblem or subsystem (Prakash and Shenoy, 2005b). Matches can be reduced by increasing subsets or decreasing loops. It should be noted that Eq. (9) is applicable for any network which contains the fixed-flowrate and/or fixed-load units. It should also be pointed out that, when the fixed-load operations are present, each should be counted both as a source and also as a sink to determine N_{S} and N_{D} in the above equations. Since the source-shift procedure is usually aimed at $N_{LP} = 0$ and $N_{ST} = 1$, a safe bet of the minimum match number should be

$$N_{\rm M} = N_{\rm S} + N_{\rm D} - 1$$
 (10)

Step 2: Perform the generalized source shifts to reduce match number until there are no opportunities for match elimination.

This step should be performed even when the target match number has already been reached because it may still be possible to form multiple subsets after source shifts. The following guidelines can be adopted to identify opportunities for removing redundant matches:

- 1. Opportunities for two-source shift:
 - (a) Basic requirements:

There are two demands in the preliminary structure which are satisfied by two separate sources. To remove any match, it is required that

- one match at most can be absent in the matching matrix if no fixed-load operations are involved in the shift, or
- two matches at most can be absent if a fixedload operation is present.

The reason for above difference is that a futile match may be generated after source shift in the latter case, and this futile match can be removed immediately.

- (b) Further requirements:
 - Two possibilities have to be considered:
 - i. The source concentrations are the same. There are three possible scenarios:
 - If two entries in the matching matrix are missing, the remaining two should be located in the diagonal or anti-diagonal



Fig. 5 - Two-source shift patterns with one absent entry.

cells and of the same value. A futile stream around a fixed-load unit can be produced with such a shift and this stream can be directly removed.

- If only one entry is missing and the other two flow rates in the diagonal or anti-diagonal cells are the same, then a source-shift candidate must be one of four options shown in Fig. 5, in which the missed entry is marked by a dashed rectangle. The total match number can be reduced from 3 to 2 after shift.
- If all entries are present, i.e., there is a loop, then the match with smaller diagonal or anti-diagonal flow rate can be eliminated by source shift (see Fig. 6).
- ii The source concentrations are different.
- One of the three conditions listed in case i must be satisfied. In addition, for the sink that receives dirtier water, its concentration should not exceed the given upper limit after shift. Note that the corresponding outlet concentration after the shift should not exceed its given upper limit either if the sink receiving dirtier water is the inlet stream of a fixed-load unit. The outlet concentration should be updated according to Eq. (2). This point will be further illustrated in Example 2.
- 2. Opportunities for three-source shift:
 - (a) Basic requirements:

Let us consider the situation when two demands are satisfied by three sources having different concentrations. One of the following two conditions should be satisfied:



Fig. 6 - Two-source shift patterns without absent entry.

- Two entries at most can be absent in the matching matrix if none of the fixed-load operations are involved in the shift. The locations of these two missing entries in the matrix must match one of the six patterns given in Fig. 7.
- Three matches at most can be absent if a fixed-load operation is present. The locations of these three missing entries should be the same as one of the two patterns given in Fig. 8.

Notice that a maximum of three existing matches can be removed after a three-source shift. Two new matches at most can be formed in the former case, while three new matches may be created and some of them may be futile in the latter case. For example, entries a, b and c in Fig. 7(a) can be removed simultaneously if $[b Sl]_{Dj} \Leftrightarrow [a Sk + c Sm]_{Di}$ while two new entries are formed after the three-source shift. As a result, the total number of matches can be reduced by one after such a shift.

(b) Further requirements:

The total number of removed matches and shift-created self-recycle streams should be larger than the number of absent entries in the original matching matrix. Since a self-recycle stream can be removed immediately and the number of newly formed entries after a shift (as shown in Figs. 7 and 8) is just the same as the number of absent entries, the further requirements here are to guarantee that the net effect of such a shift is to reduce the total match number at least by one. This point will be further elaborated in the subsequent examples.

3. Opportunities for multi-source shift:

A multi-source shift is a shift between two water demands involving more than three different sources. Note that not every demand needs to be supplied by all involved sources in this situation. Its original form was proposed by Ng and Foo (2006). Such a shift can be achieved by performing a series of two or more two-source or three-source shifts. Although each shift alone is not effective for match reduction while the combinations of two or more shifts can reduce matches. The following criteria can be adopted to identify such a shift: (a) Basic requirements:

Two demands are matched by more than three sources. Among these existing matches, it can



Fig. 7 - Three-source shift patterns with two absent entries.

be identified that multiple two- or three-source shifts could satisfy their basic requirements but not the further requirements.

- (b) Further requirements:
 - The total number of removed matches and shift-created self-recycle steams during multiple shifts should be greater than the total number of missed entries in the original matching matrix.

The above basic and further requirements of a multi-source shift can be clearly illustrated with an example concerning only the fixed-flowrate operations (see Figs. 9 and 10). This example is adopted



Fig. 8 – Three-source shift patterns with three absent entries.

from Ng and Foo (2006) and will be referred to as Example 1. Notice that there are four sources in this system and two entries are absent from the matching matrix. From these data, four possible three-source shifts can be identified, i.e.

$$[SR4]_{SK10} \Leftrightarrow \left[\frac{1}{2}FW + \frac{1}{2}SR3\right]_{SK7}$$
(11)

$$[SR4]_{SK10} \Leftrightarrow \left[\frac{2}{3} FW + \frac{1}{3} SR9\right]_{SK7}$$
(12)

$$[SR3]_{SK10} \Leftrightarrow \left[\frac{1}{3}FW + \frac{2}{3}SR9\right]_{SK7}$$
(13)

$$[SR3]_{SK10} \Leftrightarrow \left[\frac{1}{2}SR4 + \frac{1}{2}SR9\right]_{SK7}$$
(14)

These expressions could be explained by considering Eq. (11) as an example. In this particular case, since 1 t/h of SR4 is essentially the same as a mixture of 1/2 t/h of FW and 1/2 t/h of SR3, demands SK10 and SK7 can be matched interchangeably with these two equivalent sources. To reduce the number of matches, the match flow rates should be chosen so as to use up at least one of the sources involved in a three-source shift (in a way similar to the tick-off heuristic in HEN synthesis; Linnhoff and Hindmarsh, 1983). It should also be noted that, although each of them alone may not be able to reduce the number of matches, the total number of matches can be reduced by carrying out two out of

F t/hr{C ppm}	Streams	SK10 33.333{150}		SK7 5{200}	SK10 33.333{150}		SK7 5{200}	SK10 33.333{150}	SK7 5{200}
$0.323\{0\}$ 13.086 $\{100\}$ 22.857 $\{200\}$ 2.067 $\{300\}$	FW SR4 SR3 SR9	11.666 21.667	$\underbrace{\begin{array}{c} 0.323\\ 0.646\\ 0.323 \end{array}}_{0.323}$	0.323 1.42 1.19 2.067	0.323 11.02 21.99	2.066 4.133 2.067	2.066 0.867 2.067	0.323 13.086 17.857 2.067	5

Fig. 9 - Multi-source shifting sequence in Example 1.

the above four shifts in sequence. Two such shifting sequences are shown in Figs. 9 and 10 separately. Specifically, the following two three-source shifts are carried out in former table:

 $[0.646 \,\text{SR4}]_{\text{SK10}} \Leftrightarrow [0.323 \,\text{FW} + 0.323 \,\text{SR3}]_{\text{SK7}}$ (15)

 $[4.133 \text{ SR3}]_{\text{SK10}} \Leftrightarrow [2.066 \text{ SR4} + 2.067 \text{ SR9}]_{\text{SK7}}$ (16)

which are the actual form of Eqs. (11) and (14), respectively.

For the first three-source shift, the basic requirement is obviously satisfied because only entry FW - SK10 is absent from (FW, SR4, SR3, SK10, SK7). However, the further requirement is not satisfied because match FW - SK7 is removed while another new match, FW - SK10, is created after this shift. As for the second shift, both basic and further requirement are satisfied, two matches, i.e., SR4 - SK7 and SR9 – SK7, are removed and only one new match, i.e., SR9 – SK10, is created after the shift. The total number of matches is reduced from 6 to 5 although there is no reduction in total match number after the first shift. The shifted flow rates in Eq. (16) are not exactly proportional to the coefficients in Eq. (11). This is because the round error in hand calculation. The further condition is obviously satisfied here since the total number of removed matches is 3 (after two shifts), which is greater than the total number of missing entries (2). Similarly, the following two shifts are carried out in the latter table:

 $[0.4845 \text{ SR4}]_{\text{SK10}} \Leftrightarrow [0.323 \text{ FW} + 0.1615 \text{ SR9}]_{\text{SK7}}$ (17)

 $[3.81 \text{ SR3}]_{\text{SK10}} \Leftrightarrow [1.9045 \text{ SR4} + 1.9055 \text{ SR9}]_{\text{SK7}}$ (18)

which are the actual form of Eqs. (12) and (14), separately. The total number of matches is even increased by one after the first shift while decreased by two in the second shift. The net effect is that the total number of matches reduced from 6 to 5.

It should be noted that the same final result can be obtained if source shifts begin with other two candidate shifts given in Eqs. (13) and (14). It should also be made clear at this point that a similar concept 'multiple-point shift' has been discussed in Ng and Foo (2006), and such a shift can be performed in just one step. Although the multiplesource shift proposed in this work seems a little more complex and two or more shift actions are needed to accomplish the goal of match reduction, the present approach is more general in the sense that both fixed-load and fixed-flowrate units can be considered in the evolution procedure. Finally, notice that the proper precedence order for identifying source shifts should be: (1) two-source shift with the same source concentration, (2) twosource shift with different source concentrations, (3) three-source shift, and (4) multi-source shift. By following such order, the simpler candidates can be found before the more complex ones and, hopefully, all possible shifts can be enumerated.

Step 3: Target the total number of all promising configurations and judiciously generate the desired ones.In the previous step, the number of matches in the preliminary design has been reduced to the minimum level. The purpose of present step is to identify

F t/hr{C ppm}	Streams	SK10 33.333{150}		SK7 5{200}	SK10 33.333{150}		SK7 5{200}	SK10 33.333{150}	SK7 5{200}
0.323{0} 13.086{100} 22.857{200} 2.067{300}	FW SR4 SR3 SR9	11.666 21.667	<u>0.323</u> <u>0.4845</u> <u>0.1615</u>	0.323 1.42 1.19 2.067	0.323 11.1815 21.667 0.1615	$\begin{array}{r} \underbrace{1.9045}_{3.81}\\ \underbrace{1.9055}_{1.9055}\end{array}$	1.9045 1.19 1.9055	0.323 13.086 17.857 2.067	5

Fig. 10 - Another multi-source shifting sequence in Example 1.

viable two- and three-source shifts which may result in alternative configurations while keeping the freshwater consumption rate, the total number of matches and the total throughput at their lowest values, respectively. It should be noted that the multi-source shift is not considered in this step because it can be regarded as a combination of several two- and/or three-source shifts. Specifically, the following conditions must be observed before a candidate shift can be counted:

- Opportunities for two-source shift Similar to those requirements in previous step, two possibilities have to be considered:
 - (a) The source concentrations are the same. There are two possible scenarios:
 - If two entries in the matching matrix are missing, the remaining two should be located in the diagonal or anti-diagonal cells and of the same value.
 - If only one entry is missing and the other two flow rates in the diagonal or anti-diagonal cells are different, then the smaller one of diagonal and anti-diagonal flow rates can be shifted to form an alternative solution.
 - (b) The source concentrations are different.
 - One of the two conditions listed in case (a) must be satisfied. In addition, for the sink that receives dirtier water, its concentration should not exceed the given upper limit after shift. Note that the corresponding outlet concentration after the shift should not exceed its given upper limit either if the sink receiving dirtier water is the inlet stream of a fixed-load unit. The outlet concentration should be updated according to Eq. (2).
- 2. Opportunities for three-source shift
- (a) Basic requirements
 - They are the same as those listed in the previous step.
 - (b) Further requirements

The total number of removed matches after the shift should be equal to that of absent entries in the original matching matrix.

The total number of configurations $(N_{\mbox{cf}})$ can be obtained by:

$$N_{cf} = \prod_{i=1}^{K} N_i(n_{2s}, n_{3s})$$
(19)

where N_i is the number of different configurations contained in the ith *independent* source-shift set; n_{2s} and n_{3s} , respectively denote the numbers of candidate two- and three-source shifts in the ith source-shift set; K is the total number of *independent* source-shift sets. Note that N_i is a function of n_{2s} and n_{3s} . In this study, a *source-shift* set is defined as the smallest set of sources and demands among which one or more two-source or three-source shift candidate exists. The source-shift sets should be considered to be independent if they have no shared source(s) or demand(s) in the matching matrix. This concept will be further illustrated in Example 4. If n_s (= $n_{2s} + n_{3s}$) decoupled candidate shifts can be identified in set *i*, the corresponding number of alternative configurations should be:

$$N_i = \sum_{j=0}^{n_s} C_j^{n_s} \tag{20}$$

where

$$C_j^{n_s} = \frac{n_s!}{(n_s - j)!j!}$$
(21)

and $C_0^{n_s} = 1$. Notice that two or more shifts are considered to be *decoupled* if none of them can be replaced with a combination of the others and they can all be performed in sequence. On the other hand, all alternative configurations can only be exhaustively enumerated in a trial-and-error process if the identified candidate shifts are coupled. Note that $N_{cf} = 1$ if there is no source-shift set at all in the matching matrix corresponding to the optimal solution. It should be made clear that an alternative network configuration is counted in N_{cf} only if it has at least one unique match or stream.

In this work, it is required that the preliminary network features minimum freshwater usage. The minimum match number can be achieved by implementing Steps 0–2, while the minimum total throughput can be realized by carrying out Steps 0 and 2 according to the proposed stream deletion conditions in Section 4. Therefore, the networks obtained before Step 3 are already optimal in terms of the aforementioned three criteria. It should be emphasized that every alternative solution can be found and generated if all candidate shifts are fully explored in Step 3. This is due to the fact that source shifts are the only cause for more than one alternative configuration.

6. Applications

To demonstrate the applicability and effectiveness of the proposed procedure, three different types of problems have been studied.

6.1. Fixed-load problems

In the matching matrix, the inlet and outlet water streams of each fixed-load operation should be regarded as demand and source, respectively. On the other hand, the freshwater should be treated only as a source and the effluent as a sink or demand. Three examples are presented below to illustrate the proposed evolution procedure.

Example 2. The process data adopted in the present example are taken from Wang and Smith (1994) (see Table 1). The

Table 1 – Process data of Example 2.							
¯C ⁱⁿ (ppm)	$\overline{C}^{out}(ppm)$	Mass load (kg/h)	F ^{lim} (t/h)				
0	100	2	20				
50	100	5	100				
50	800	30	40				
400	800	4	10				
	Process data $\overline{C}^{in}(ppm)$ 0 50 50 400	$\overline{C}^{in}(ppm)$ $\overline{C}^{out}(ppm)$ 01005010050800400800	Process data of Example 2. $\overline{C}^{in}(ppm)$ $\overline{C}^{out}(ppm)$ Mass load (kg/h)0100250100550800304008004				



Fig. 11 - Preliminary design for Example 2.



Fig. 12 – Improved preliminary design for Example 2.

minimum freshwater consumption in this case is 90 t/h, a preliminary design can be found in Fig. 11, notice that the selfrecycle streams in the solution have been removed to reduce the throughput (Dunn and Wenzel, 2001). According to the stream deletion conditions, we can find that the reuse stream from P1 to P2 is futile, and it should be removed to further reduce the throughput of P2. The improved preliminary design is provided in Fig. 12 and its matching matrix is given in Fig. 13. The first row of this matching matrix represents a freshwater (S0) source, whereas the last column is the wastewater (WW). The actual concentration of demands are given in blue and boldfaced number if they are less than their maximum values. Here, D1 and S1 represent the inlet and outlet stream of unit P1, respectively, and D2–D4 and S2–S4 have similar meaning. Such conventions are also adopted in Examples 3 and 4. Following is a summary of the implementation steps of the proposed procedure:

Step 1: Target the match number as:

$$N_{M} = N_{S} + N_{D} - 1 = 5 + 5 - 1 = 9$$

Since there are 9 interconnections in the improved primary network, it would appear that it is already optimal.

- Step 2: By examining Fig. 13, a candidate two-source shift between sinks D3 and WW can be found and is already marked by a dashed rectangle, and a match can be reduced according to the condition shown in Fig. 5(c). (S0, S2, D2, D3) is not a two-source shift candidate although the actual concentration in sink D2 is less than its maximum value of 50 ppm and the basic requirements are satisfied. This is due to the fact that demand D2 and source S2 here are the inlet and outlet streams of unit P2, respectively, i.e., their concentrations are not independent but constrained by Eq. (2). Thus, the concentrations of S2 should be raised to 140 ppm (larger than its upper limit) after carrying out the shift $[20 \text{ S0}]_{D2} \Leftrightarrow [20 \text{ S2}]_{D3}$. Similarly, (S0, S2, D4, D3) is not a two-source shift candidate either. It should be noted that demands in Fig. 13 are not arranged completely according to the ascending order of their maximum inlet concentrations. This practice is adopted for the purpose of showing the candidate two-source shifts more clearly. The resulting matching matrix after shift is given in Fig. 14. Notice that the number of interconnections is now reduced to 8, which is one match less than the target of 9. This is due to the fact that the system consists of two subsets instead of one. Specifically, it is clear from Fig. 14 that (S0, S1, D1, D2, D3) form a subset and the remaining sources and sinks represent another one.
- Step 3: According to the requirements for source shift candidates (listed in Step 3), no candidate shifts can be identified and no source-shift sets can be found in Fig. 14. Consequently, there is only one optimal configuration for this example and this network is the same as the one reported by Prakash and Shenoy (2005a) and also by Li and Chang (2011b).

Example 3. This example is adopted from Olesen and Polley (1997) (see Table 2), in which the minimum freshwater consumption rate can be determined to be 157.143 t/h (Olesen and Polley, 1997; Prakash and Shenoy, 2005a; Savelski and Bagajewicz, 2001). Two alternative preliminary networks can be found in the literature, i.e., Fig. 15 and 16. The former solution (Savelski and Bagajewicz, 2001) satisfies the necessary conditions of optimality (Savelski and Bagajewicz, 2000) and also consumes the least amount of freshwater. The latter (Prakash and Shenoy, 2005a) features the minimum levels of

F t/hr{C ppm}	Streams	D1 20{0}	D2{50} 50{ <mark>0</mark> }	D4{400} 5.71{100}	D3 40{50}	$WW\{\infty\}$ 90 $\{455.5\}$
90{0} 20{100} 50{100} 40{800} 5.71{800}	S0 S1 S2 S3 S4	20	50	5.71	<u>20</u> 20	20 20 20 40 5.71

Fig. 13 - Improved preliminary design represented as matching matrix for Example 2.

F t/hr{C ppm}	Streams	D1 20{0}	D2{50} 50{ <mark>0</mark> }	D4{400} 5.71{ <mark>100</mark> }	D3 40{50}	$WW\{\infty\}$ 90{455.5}
$90\{0\}$ 20{100} 50{100} 40{800} 5.71{800}	S0 S1 S2 S3 S4	20	50	5.71	20 20	44.29 40 5.71

Fig. 14 – Final matching matrix for Example 2.

F t/hr{C ppm}	Streams	D1{25} 25 { <mark>0</mark> }	D2 {25} 50{ <mark>0</mark> }	D3 22.857{25}	D4 {50} 70 {28.57}		D5 40 {50}	D6{400} 5.714{ <mark>100</mark> }	WW{∞} 157.143
$\begin{array}{c} 157.143\{0\}\\ 25\{80\}\\ 50\{100\}\\ 70\{100\}\\ 22.857\{200\}\\ 40\{800\}\\ 5.714\{800\}\end{array}$	FW S1 S2 S4 S3 S5 S6	25	50	17.143 5.714	45	25 25 20	20 20	5.714	50 38.572 22.857 40 5.714

Fig. 15 - Preliminary design I represented as matching matrix for Example 3.

F t/hr{C ppm}	Streams	D1{25} 25 { <mark>0</mark> }	D2 {25} 50 <mark>{0</mark> }	D4 {50} 50 { <mark>0</mark> }	D3 22.857{25}		D5 40 {50}	D6{400} 5.714{ <mark>100</mark> }	WW{∞} 157.143
$157.143\{0\}$ $25\{80\}$ $50\{100\}$ $50\{100\}$ $22.857\{200\}$ $40\{800\}$ $5.714\{800\}$	FW S1 S2 S4 S3 S5 S6	25	50	50	15.714 7.143	$\begin{array}{c} 1.4285\\ \hline 7.143\\ \hline 5.714 \end{array}$	16.429 17.857 5.714	5.714	44.286 44.286 22.857 40 5.714

Fig. 16 – Preliminary de	sign II represented	as matching matri	x for Example	3
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freshwater usage and minimum total throughput (193.571 t/h). This example is used to shown different preliminary networks have no effect on obtaining all promising alternative solutions.

Table 2 – Process data of Example 3.							
Unit no.	\overline{C}^{in} (ppm)	[¯] C ^{out} (ppm)	Mass load (kg/h)	F ^{lim} (t/h)			
P1	25	80	2	36.36			
P2	25	100	5	66.67			
РЗ	25	200	4	22.86			
P4	50	100	5	100			
P5	50	800	30	40			
Р6	400	800	4	10			

Because there is no futile streams in preliminary designs, step 0 is skipped here and the other proposed steps are implemented as follows:

Step 1: The target number of interconnections is:

$$N_{\rm M} = N_{\rm S} + N_{\rm D} - 1 = 7 + 7 - 1 = 13$$

Since the numbers of interconnections in Figs. 15 and 16 are both 14, it is reasonable to expect that one match in each case can be eliminated.

Step 2: Only one candidate three-source shift can be identified in each preliminary network and it has been marked by dashed rectangle in Figs. 15 and 16. The shift between D4 and D5 in Fig. 15 can create a selfrecycle stream around unit P4 as shown in Fig. 17,

Streams	D1{25} 25 {0}	D2 {25} 50{0}	D3 22.857{25}	D4 $\{50\}$ 70 $\{28.57\}$	D5 40 {50}	D6{400} 5.714{ <mark>100</mark> }	WW {∞} 157.143
FW S1	25	50	17.143	50	$\frac{15}{25}$		
S2 S4 S3 S5			5.714	20		5.714	$50 \\ 38.572 \\ 22.857 \\ 40 \\ 5.714$
	Streams FW S1 S2 S4 S3 S5 S5	Streams D1{25} 25 {0} FW 25 S1 52 S4 53 S5 56	$\begin{array}{c cccc} \text{Streams} & D1\{25\} & D2 \{25\} \\ 25 \{0\} & 50\{0\} \\ \hline \\ FW & 25 & 50 \\ S1 \\ S2 \\ S4 \\ S3 \\ S5 \\ S6 \\ \hline \end{array}$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Streams D1{25} 25 {0} D2 {25} 50{0} D3 22.857{25} D4 {50} 70 {28.57} FW 25 50 17.143 50 S1 S2 53 5.714 20 S3 S5 S6 56 50	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $

Fig. 17 – Promising design I after shift for Example 3.

while a shift between D3 and D5 in Fig. 16 can reduce a match as shown in Fig. 18. Notice that the match target of 13 can be achieved in both cases (after removing the self-recycle stream in Fig. 17) and, furthermore, the total throughput is also reduced by removing the self-recycle stream.

Step 3: From Fig. 18, one can see that there is only one candidate source-shift set, i.e. (D3, D6, WW, S2, S4), which is also marked by a dashed rectangle. The involved match flow rates are marked in blue. Three alternative two-source shifts are included, i.e.

 $[5.714S2]_{D3} \Leftrightarrow [5.714S4]_{WW}$ (22)

$$[5.714S4]_{D6} \Leftrightarrow [5.714S2]_{WW}$$
 (23)

$$[5.714S2]_{D3} \Leftrightarrow [5.714S4]_{D6}$$
 (24)

Only two of the above three shifts are decoupled since Eq. (24) can be realized by carrying out the operations specified in Eqs. (22) and (23). Thus, $n_s = 2$ and the corresponding alternative configurations can be generated by performing the shift in Eq. (22) or (23) alone, or both shifts.

The total number of alternative configurations according to Eq. (20) is:

$$N_{cf} = N_1 = \sum_{j=0}^{2} C_j^2 = 4$$
(25)

in which C_0^2 represents the base case when no shifts are performed.

It should pointed out that the same target on the total number of alternative solutions can be obtained if Fig. 17 (after removing the self-recycle stream, i.e. subtracting 20 t/h from both D4 and S4 simultaneously and removing the entry of 20 from the matching matrix) is analyzed. Fig. 17 (after removing the self-recycle stream) can be obtained if the shift indicated by Eq. (22) is performed in Fig. 18. The other two promising configurations can be generated easily, but are not presented here for brevity. It can be easily checked that all alternative promising solutions characterized by freshwater usage of 157.143 t/h, total number of connections of 13 and total throughput of 193.571 t/h. Notice that these results are just as good as those reported by Li and Chang (2011b).

Example 4. Table 3 shows the design specifications of a water network involving 10 fixed-load operations. The freshwater usage level has been targeted to be 165.9 t/h, the preliminary design for this example is adopted from Bagajewicz and Savelski (2001) (see Figs. 19 and 20), which features the minimum match number (22) and also the above-mentioned minimum freshwater consumption rate.

Step 0 is skipped because of there is no futile streams in Fig. 19 and following are other evolution steps:

F t/hr{C ppm}	Streams	D1{25} 25 { <mark>0</mark> }	D2 {25} 50{ <mark>0</mark> }	D4 {50} 50 { <mark>0</mark> }	D3 22.857{25}	D5 40 {50}	D6{400} 5.714{ <mark>100</mark> }	WW{∞} 157.143
$\begin{array}{c} 157.143\{0\}\\ 25\{80\}\\ 50\{100\}\\ 50\{100\}\\ 22.857\{200\}\\ 40\{800\}\\ 5.714\{800\}\end{array}$	FW S1 S2 S4 S3 S5 S6	25	50	50	17.143	15 25	5.714	44.286 44.286 22.857 40 5.714

Fig. 18 - Promising design II after shift for Example 3.



Fig. 19 - Preliminary design for Example 4.

F t/hr {C ppm}	Streams	D1{25} 25 { <mark>0</mark> }	D2{25} 32 { 0 }	D4{50} 30 { <mark>0</mark> }	D8 10 {0}	D3 16.5 {25}	D9 37.4 {50}	D5 15 {50}	D10{150} 41.9 {144.9}	$\begin{array}{c} \text{D6 } \{400\} \\ 9.2 \\ \{\textbf{256.5}\} \end{array}$	D7{400} 6.7 { <mark>300</mark> }	WW{∞} 165.9
$165.9\{0\}\\25\{80\}\\32\{90\}\\30\{100\}\\10\{100\}\\22.8\{200\}\\80\{300\}\\41.9\{300\}\\6.7\{600\}\\40\{800\}\\9.2\{800\}$	FW S1 S2 S4 S3 S9 S10 S7 S5 S6	25	32	30	10	16.5 6.3	37.4 25.7 6.9 10	15 25	23.1 18.8	4 5.2	6.7	74.8 35.2 6.7 40 9.2

Fig. 20 - Preliminary design represented as matching matrix for Example 4.

Step 1: The target match number is:

```
N_{\rm M} = N_{\rm S} + N_{\rm D} - 1 = 11 + 11 - 1 = 21
```

Table 3 – Process data of Example 4.										
Unit no.	[¯] C ⁱⁿ (ppm)	[¯] C ^{out} (ppm)	Mass load (kg/h)	F ^{lim} (t/h)						
P1	25	80	2.0	36.36						
P2	25	90	2.88	44.31						
РЗ	25	200	4.0	22.86						
P4	50	100	3.0	60						
P5	50	800	30	40						
P6	400	800	5.0	12.5						
P7	400	600	2.0	10						
P8	0	100	1.0	10						
Р9	50	300	20.0	80						
P10	150	300	6.5	43.33						

Thus, it may be possible to reduce the match number by 1.

- Step 2: A loop connecting sources FW and S2 and demands D3 and D9 can be identified in Fig. 20 and it is marked by a dotted rectangle. Since this loop cannot be broken by source shift without incurring penalty in freshwater usage and, also, there are no candidate two- or three-source shifts which can further simply the preliminary network, the number target obtained in Step 1 is therefore relaxed by 1.
- Step 3: Two independent source-shift sets (marked by dashed rectangles) can be identified in Fig. 20. One is (S4, S8, D9, D10) and only one candidate two-source shift can be found, i.e. [10S8]_{D9} ⇔ [10S4]_{D10}, while the other is (S9, S10, D6, D7, WW) and there are two decoupled shifts, i.e.

```
[5.2S9]<sub>D6</sub> ⇔ [5.2S10]<sub>WW</sub>
```

Table 4 – Pro	Table 4 – Process data of Example 5.									
	Sources			Demands						
ID no.	Flow rate F _i (t/h)	Concentration C _i (ppm)	ID no.	Flow rate F _j (t/h)	Concentration C _j (ppm)					
S1	50	50	D1	50	20					
S2	100	100	D2	100	50					
S3	70	150	D3	80	100					
S4	60	250	D4	70	200					

F t/hr{C ppm}	Streams	D1 50{20}	D2 100{50}		D3 80{100}	D4 70{200}	$WW\{\infty\}\ 50\{200\}$
$70\{0\}\ 50\{50\}\ 100\{100\}\ 70\{150\}\ 60\{250\}$	S0 S1 S2 S3 S4	30 20	35 30 35	5 15 10	5 65 10	[35 35	$\frac{25}{25}$ 25

Fig. 21 - Preliminary network represented as matching matrix for Example 5.

$$[6.7S10]_{D7} \Leftrightarrow [6.7S9]_{WW} \tag{27}$$

Because these two sets are independent and the total alternative configurations of this example would be

$$N_{cf} = N_1 \times N_2 = \left(\sum_{j=0}^1 C_j^1\right) \times \left(\sum_{k=0}^2 C_k^2\right) = 2 \times 4 = 8(28)$$

Note that this number can be obtained before actually generating all promising alternative solutions (Li and Chang, 2011b), and a desired network can be easily obtained by judiciously carrying out the identified source shifts.

6.2. Fixed-flowrate problem

Example 5. Let us consider the fixed-flowrate problem studied by Polley and Polley (2000). There are four internal sources and four internal demands in this water network and their process data can be found in Table 4. The minimum freshwater consumption rate and wastewater discharge rate were found to be 70 and 50 t/h, respectively (Prakash and Shenoy, 2005a). Prakash and Shenoy (2005b) generated the preliminary network in Fig. 21. As shown, there are 12 connections in this network and the minimum level of freshwater usage is achieved. The implementation steps of the source-shift procedure are outlined below:

Step 1: The minimum number of matches is:

$$N_{\rm M} = N_{\rm S} + N_{\rm D} - 1 = 5 + 5 - 1 = 9$$

Thus, it may be possible to remove 12 - 9 = 3 matches.

Step 2: On the basis of the requirements specified in the proposed source-shift procedure, one candidate two-source shift (between demands D4 and WW) and one candidate three-source shift (between demands D2 and D3) can be identified in the preliminary network. The shifted water flow rates are also shown in Fig. 21. After performing these two candidate shifts, the number of matches in the evolved network (which is referred to as *Design I*) can be reduced to 10. The corresponding matching matrix is shown in Fig. 22.

$F t/hr{C ppm}$	Streams	D1 50{20}	D2 100{50}	D3 80{100}	D4{200} 70{ <mark>164.3</mark> }	$\begin{array}{l} WW\{\infty\}\\ 50\{\textbf{250}\}\end{array}$
$70\{0\}\ 50\{50\}\ 100\{100\}\ 70\{150\}\ 60\{250\}$	S0 S1 S2 S3 S4	130 120	10 49 20 30 10 20 55hift 2	{Loop] 80 {Shift 1]	60 10	50

Fig. 22 - Design I represented as matching matrix for Example 5.

F t/hr{C ppm}	Streams	D1 50{20}		D2 100{50}	D3 80{100}	D4{200} 70{ <mark>164.3</mark> }	WW $\{\infty\}$ 50 $\{250\}$
$70\{0\}$ $50\{50\}$ $100\{100\}$ $70\{150\}$ $60\{250\}$	S0 S1 S2 S3 S4	40 10	$\underbrace{\frac{3.33}{\underline{10}}}_{\underbrace{6.67}}$	30 50 10 10	80	60 10	50

Fig. 23 - Design II represented as matching matrix for Example 5.

F t/hr{C ppm}	Streams	D1 50{20}	D2 100{50}	D3 80{100}	$\begin{array}{c} {\rm D4\{200\}}\\ {\rm 70\{164.3\}}\end{array}$	$\begin{array}{l} WW\{\infty\}\\ 50\{250\}\end{array}$
$70\{0\}\ 50\{50\}\ 100\{100\}\ 70\{150\}\ 60\{250\}$	S0 S1 S2 S3 S4	43.33 6.67	26.67 50 20 3.33	80	60 10	50

Fig. 24 –	Design III	represented	as matching	matrix for	Example 5.
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Notice that the match number in this modified network is larger than the target value. This is due to the fact that a loop, i.e. $([30S0]_{D1}, [40S0]_{D2}, [30S1]_{D2}, [20S1]_{D1})$, cannot be broken by source shift.

Step 3: According to the proposed source-shift procedure, only one source-shift set can be identified, i.e. (S0, S1, S2, S3, D1, D2), and two *coupled* candidate shifts are included, i.e.

$$[20S1]_{D1} \Leftrightarrow [10S0 + 10S2]_{D2}$$
 (29)

$$[20S1]_{D1} \Leftrightarrow [13.33S0 + 6.67S3]_{D2}$$
(30)

They are marked by dashed rectangles in Fig. 22. Since both shifts involve S1 and will tick it off, it is obvious that these two candidate shifts can not be carried out in order. So, the former shift is chosen in this example. After performing the shift shown in Fig. 22, an alternative network (i.e., Design II in Fig. 23) can be obtained. By inspecting Design II, a new candidate three-source shift can be found:

$$[10S2]_{D1} \Leftrightarrow [3.33S0 + 6.67S3]_{D2}$$
 (31)

The resulting design after shift is shown in Fig. 24. It should be noted that this design can also be produced

S F t/hr {C ppm}	treams	P1 _{in} 20 {0}	$P2_{in}\{50\}\50\{0}\}$	D1 50 {20}	$P3_{in} \\ 40 \\ \{50\}$	D2 100 {50}	D3 80 {100}	$P4_{in}$ {400} 5.714 {100}	D4 70 {200}	WW{∞} 135
$155\{0\}$ $50\{50\}$ $20\{100\}$ $50\{100\}$ $100\{100\}$ $70\{150\}$ $60\{250\}$ $40\{800\}$ $5.714\{800\}$	$\begin{array}{c} \mathrm{FW} \\ \mathrm{S1} \\ P1_{out} \\ P2_{out} \\ \mathrm{S2} \\ \mathrm{S3} \\ \mathrm{S4} \\ P3_{out} \\ P4_{out} \end{array}$	20	50		5 5 10 30 5 5 5	50 50	80	5.714		9.286 35 35 25 35 40 5.714

F t/hr {C ppm}	Streams	$P1_{in}$ 20 $\{0\}$	$P2_{in}\{50\}\50\{0}\}$	D1 50 {20}	P3 _{in} 40 {50}	D2 100 {50}	D3 80 {100}	$P4_{in} \{400\} \\ 5.714 \\ \{100\}$	D4 70 {200}	WW{∞} 135
$\begin{array}{c} 155\{0\}\\ 50\{50\}\\ 20\{100\}\\ 100\{100\}\\ 50\{100\}\\ 70\{150\}\\ 60\{250\}\\ 40\{800\}\\ 5.714\{800\}\end{array}$	$\begin{array}{c} \mathrm{FW} \\ \mathrm{S1} \\ \mathrm{P1}_{out} \\ \mathrm{S2} \\ \mathrm{P2}_{out} \\ \mathrm{S3} \\ \mathrm{S4} \\ \mathrm{P3}_{out} \\ \mathrm{P4}_{out} \end{array}$	20	50	35 10 5	40	50 	80	5.714	70	9.286 20 50 40 5.714

Fig. 26 - Matching matrix after source shifts for Example 6.

by applying the shift specified in Eq. (30) to Design I. Since no new candidate shifts can be identified at this point, the evolution procedure should be terminated and, thus, the total number of alternative configurations is 3. These designs are as good as those reported ones (Das et al., 2009; Li and Chang, 2011b; Poplewski et al., 2010; Prakash and Shenoy, 2005b) while different methods are adopted as reviewed in the introduction section.

Finally, it should be made clear that the available loopbreak and/or path-relaxation methods (Das et al., 2009; Ng and Foo, 2006; Prakash and Shenoy, 2005b) can be easily applied to the aforementioned promising solutions to generate various different versions of the 'near-optimal' designs at designer's will. These possibilities are not further discussed here for the sake of brevity.

6.3. Hybrid problem

Example 6. The process data of Examples 2 and 5 are combined to form a hybrid problem in this case. The minimum freshwater target is 155 t/h, and a preliminary network has been produced by Prakash and Shenoy (2005a), i.e., see Fig. 25.

Step 0 is skipped because of no futile streams and following are other evolution steps:

Step 1: The target match number can be computed as follows:

 $N_{M} = N_{S} + N_{D} - 1 = 9 + 9 - 1 = 17$

Since the number of interconnections in the primary network is 19, there may be opportunities for reducing the total match number by 2 via breaking loops.

Step 2: By carrying out the two candidate shifts marked by the dashed rectangles in Fig. 25, the match number can be lowered by 2 and the resulting network is given in Fig. 26. Notice that one extra match is removed. This is due to the fact that an additional subset (S3, D4) is formed in the evolved solution.

Step 3: Only one source-shift set, i.e. (P1_{out}, S2, D1, D3, P4_{in}, WW), can be identified in Fig. 26 and there are three decoupled two-source shifts:

 $[5P1_{out}]_{D1} \Leftrightarrow [5S2]_{WW}$ (32)

$$[5.714P1_{out}]_{P4_{in}} \Leftrightarrow [5.714S2]_{WW}$$
(33)

$$[9.286P1_{out}]_{WW} \Leftrightarrow [9.286S2]_{D3}$$
 (34)

An alternative configuration can be generated by performing

- any of them alone,
- a combination of any two in sequence, or
- all of them in sequence.

Therefore, the total number of possible combinations of these shifts is:

$$N_{cf} = N_1 = \sum_{j=0}^3 C_j^3 = 8$$

These 8 promising alternative solutions can be judiciously generated if needed. They are *all* solutions that were found by mathematical programming based method (Li and Chang, 2011b). It should be pointed out that the shifted match flow rate may be affected by the prior shifts. For example, the flow rate actually transferred in the shift indicated by Eq. (34) should be 9.286+5=14.286 t/h rather than 9.286 t/h if it is performed immediately after the shift indicated by Eq. (32) (which changes the flow rate of match $[P1_{out}]_{WW}$). Otherwise, the total number of interconnections will be increased by 1.

7. Conclusions

A systematical method has been developed in this work to judiciously generate the desired promising alternative configurations of any single-contaminant water-using system from a preliminary design. The proposed manual evolution strategy has been tested in a series of extensive case studies. Based on the test results obtained so far, one can conclude that

- 1. The existence of alternative configurations can almost always be attributed to source shifts;
- The minimum number of interconnections in an promising water network can be approximately predicted on the basis of graph theory;
- The generalized shift guidelines have been proven to be effective and more general than the available ones;
- 4. The total number of all promising alternative configurations of water network can be targeted and all solutions can be generated by our proposed evolution procedure.

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