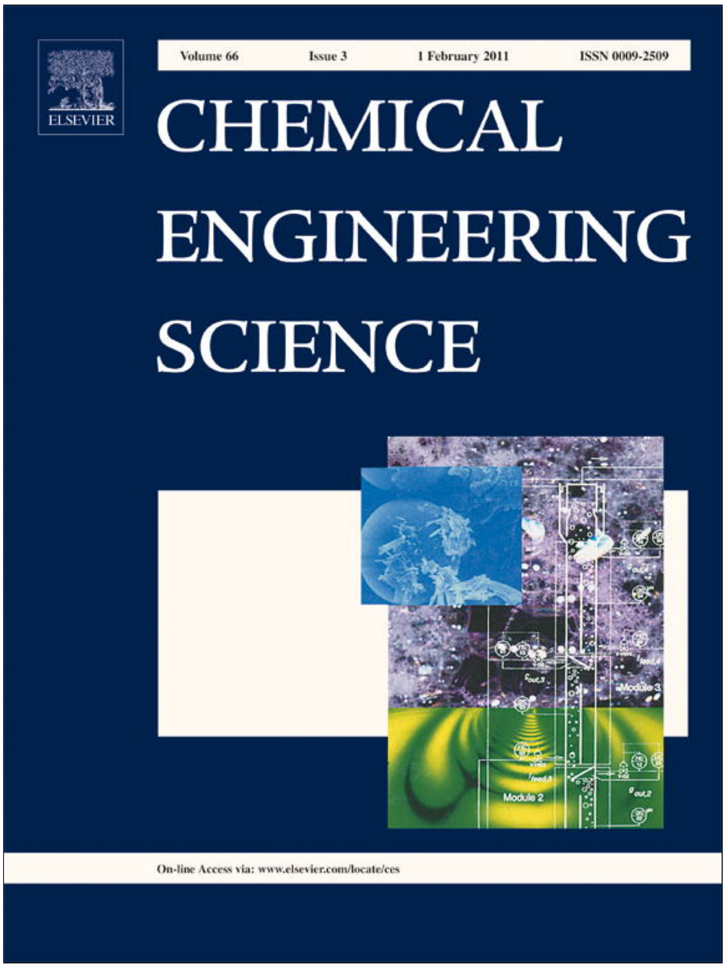

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Heuristic evolution strategies for simplifying water-using networks with multiple contaminants

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ABSTRACT

In designing a realistic water-using network with more than one contaminant, it is often desirable to obtain a simple structure so as to achieve high levels of controllability, operability, and safety. Based on any given preliminary design, the proposed heuristic evolution procedure can be systematically applied to produce an improved network with fewer interconnections, less total throughput and near minimum freshwater usage. Specifically, the minimum interconnection number is first targeted on the basis of graph theory and, then, three basic evolution strategies, i.e., loop breakage, two-source shift and path relaxation, can be utilized to strive for the number target. The required calculations in this procedure can be easily realized with Microsoft Office Excel or a hand calculator. Two examples are presented in this paper to illustrate the implementation steps and to demonstrate the effectiveness of the proposed approach.

1. Introduction

In designing a realistic water-using network (Prakash and Shenoy, 2005a), it is in general advantageous to aim for a simple structure with the fewest possible interconnections since this feature is closely associated with high levels of controllability, operability, and safety (Das et al., 2009). Two distinct approaches were taken for this purpose. One is to simplify a preliminary network with heuristic evolution strategies based on source shift (Prakash and Shenoy, 2005b), loop breakage (Das et al., 2009) and path relaxation (Ng and Foo, 2006), while the other is essentially model based (Bagajewicz and Savelski, 2001; Das et al., 2009; Faria and Bagajewicz, 2010; Li and Chang, accepted for publication; Poplewski et al., 2010). The former is the focus of present study.

It should be pointed out that the available evolution strategies were primarily developed for the fixed-flowrate operations (Polley and Polley, 2000). The inlet and outlet streams of every fixed-load unit in the previous works were considered as *independent* demand and source, while the material-balance relation between their flow rates was totally ignored (Das et al., 2009; Ng and Foo, 2006; Prakash and Shenoy, 2005b). This treatment is fundamentally flawed since (1) the inlet and outlet flow rates of every fixed-load operation are not necessarily equal due to water loss or gain and (2) these flow rates should be allowed to vary as long as the given load is removed (Prakash and Shenoy, 2005a). On the other hand, it should also be noted that all previous studies were only concerned with single-contaminant systems. Since multiple contaminants are almost always present in the industrial water networks (Alva-Argaez et al., 2007; Doyle and Smith, 1997; Li and Chang, 2007), there is a definite need to develop generalized evolution strategies for practical applications.

2. Heuristic evolution strategies

To obtain simpler configurations from a preliminary one, the minimum number of interconnections must be first established as a design target. As pointed out by Prakash and Shenoy (2005b), any water-using network can be characterized by a bipartite graph with nodes denoting the water streams (sources and demands) and edges denoting the matches. The number of matches (N_M) can then be calculated according to Euler's network theorem:

$$N_M = N_S + N_D + N_{LP} - N_{ST} \qquad (1)$$

where N_S and N_D represent the numbers of water sources and demands respectively; N_{LP} is the number of independent loops; N_{ST} is the number of subset. Clear definitions of a loop and subset have been given by Prakash and Shenoy (2005b). Note that, when the fixed-load operations are present, each should be counted both as a

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source and also as a sink to determine N_S and N_D in the above equations.

Since the evolution procedure is usually aimed at $N_{LP}=0$ and $N_{ST}=1$, a safe bet of the minimum match number should be

$$N_M^{Target}=N_S+N_D-1 \tag{2}$$

The number of loops in the preliminary networks should be larger than or equal to the difference between the actual number of interconnections and the targeted value. Specifically, the number of loops is just equal to the difference if $N_{ST}=1$, and it will be larger than the difference if $N_{ST}>1$.

Having established the number target, the improved configurations can then be evolved from the preliminary network according to the following heuristic strategies:

***Strategy* 1: Loop breakage.** According to Das et al. (2009), the matches in a loop can be partitioned into two groups. A loop may be "broken" by *flow perturbation* accordingly, i.e., the flow rate of every match in one group may be raised by an *equal amount* while each in the other group reduced by the same amount. In order to reduce a match in the loop, i.e., break the loop, this amount should be the minimum flow rate in either group.

Notice that loop breakage must not cause violation(s) of the concentration constraint(s) at each involved demand or sink. For a fixed-load unit, its outlet concentration should be updated on the basis of mass balance if its inlet stream is involved in the loop-breaking operation. This updated outlet concentration may exceed the upper bound even when the inlet concentration is feasible after loop breakage. In this situation, an additional evolution step (e.g. another loop breakage or two-source shift) is required to counteract the incurred concentration violation.

***Strategy* 2: Two-source shift.** A candidate of two-source shift can be identified according to the following two criteria:

- Two demands are satisfied by two different sources and only one entry is missing in the corresponding positions in *matching matrix* (Das et al., 2009; Prakash and Shenoy, 2005b).
- A fixed-load operation is involved in the shift and its outlet concentrations do not reach their maximums.

The shift is feasible if (1) a self-recycle stream around the fixed-load unit is formed by shifting the smaller flow rate in the diagonal or anti-diagonal entries of the matching matrix and (2) no inlet concentration violations occur in the two demands. The resulting self-recycle stream can be removed immediately to reduce the throughput of the fixed-load unit and its capital cost.

Similarly, two-source shift should not cause violation(s) of the concentration constraints at each involved demand or sink either. The outlet concentration limits of a fixed-load unit may be exceeded although there is no violation at the inlet after shift. Another evolution step (e.g., loop breakage or two-source shift) may be needed to render the shift feasible. This strategy will be later illustrated with examples.

***Strategy* 3: Path relaxation.** A path is a series of connected matches which starts and ends at external source and sink respectively. Das et al. (2009) pointed out that the matches in a path can also be divided into two groups. One group should include external source, external sink and other source-demand matches, while the other group involves only internal source-demand matches. The match with the minimum flow rate in the latter group can be eliminated by flow perturbation. This strategy will also be illustrated by examples in the subsequent section.

Note that, since only strategy 3 incurs freshwater penalty, the first two should be considered first. To keep the resulting design changes as small as possible, it is preferable to start by applying the strategy which can eliminate a match with the lowest flow rate and the fewest affected matches.

3. Applications

To demonstrate the effectiveness of the proposed strategies, two examples are presented below:

3.1. Example 1

The process limiting data from Doyle and Smith (1997) are listed in Table 1. Four fixed-load operations and three contaminants are present in this system. Only one external source (which can be viewed as a pure-water supply with no contaminants) and one external demand are available for this example. The minimum freshwater consumption rate was found to be 81.22 t/h (Doyle and Smith, 1997). An optimal solution generated by our previous model (Li and Chang, 2007) is shown in Table 2, and it is adopted here as the preliminary network. Following is a summary of the subsequent evolution steps:

Step 1: Target the match number according to Eq. (2).

$$N_M^{Target}=N_S+N_D-1=5+5-1=9$$

Since there are 10 interconnections in the preliminary network, it is possible to remove one match.

Step 2: Analyze the network structure on the basis of *matching matrix*.

Two loops can be identified in Table 2 and they are marked respectively in cyan and green colors with a common element in red. In addition, there are two subsets in the preliminary network, i.e., (FW, D1 and D2) form one subset and the remaining sources and demands are included in the other one. Thus, there are two candidates for loop breakage.

Step 3: Break loop(s) without violating concentration constraints.

The second loop (in green) is first considered because match S2–WW has the smallest flow rate, i.e., 0.607 t/h. Loop breaking is feasible in this case because (1) the concentration of source S2 is less than that of S3 for each contaminant and (2) none of the concentration constraints at demand D4 are violated after replacing 0.607 t/h of source S3 with S2 at the same flow rate. Note that the concentrations of source S4 should be changed accordingly after the loop breakage. The evolved solution is provided in Table 3.

The first loop (in cyan) is then broken by eliminating match S2–D3. Since the contaminant concentrations of both S1 and S2 are less than the corresponding maximum allowable concentrations of D3, any combination of these two sources cannot exceed the same

Table 1
Process limiting data of Example 1.

Unit no.	Limiting F (t/h)	Contaminant	$\overline{C}_{u,k}^{in}$ (ppm)	$\overline{C}_{u,k}^{out}$ (ppm)
1	34	a	0	160
		b	0	450
		c	0	30
2	75	a	200	300
		b	100	270
		c	500	740
3	20	a	600	1240
		b	850	1400
		c	390	1580
4	80	a	300	800
		b	460	930
		c	400	900

Table 2
Matching matrix of Example 1.

{C }	F	Streams	D1 34 {0,0,0}	D2{200,100,500} 47.22 {0,0,0}	D3{600,850,390} 17.154 {159.6, 385.7, 155.4}	D4{300,460,400} 65.0 {177.0, 351.6, 284.7}	WW 81.22 {809.4, 943.7, 1019.7 }
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S1			*11.03*	*22.97*	
{158.8,270.0,381.2}	47.22	S2			*6.124*	*40.491*	*0.607*
{905.8,1027.0,1542.8}	17.154	S3				*1.543*	*15.611*
{792.3,930.0,900.0}	65.0	S4					65.0

Table 3
Evolved network after loop 2 break of Example 1.

{C }	F	Streams	D1 34 {0,0,0}	D2{200,100,500} 47.22 {0,0,0}	D3{600,850,390} 17.154 {159.6, 385.7, 155.4}	D4{300,460,400} 65.0 {170.0, 344.5, 273.8}	WW 81.22
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S1			*11.03*	*22.97*	
{158.8,270.0,381.2}	47.22	S2			*6.124*	*41.098*	
{905.8,1027.0,1542.8}	17.154	S3				0.936	16.218
{785.4,923.0,889.2}	65.0	S4					65.0

Table 4
Evolved network after loops 2 and 1 break of Example 1.

{C }	F	Streams	D1 34 {0,0,0}	D2{200,100,500} 47.22 {0,0,0}	D3{600,850,390} 17.154 {160, 450, 30}	D4{300,460,400} 65.0 {170.0, 328.6, 305.2}	WW 81.22
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S1			*17.154*	*16.846*	
{158.8,270.0,381.2}	47.222	S2				47.222	
{906.4,1091.4,1417.8}	17.154	S3				*0.936*	*16.218*
{785.3,907.0,920.5}	65.0	S4					*65.0*

upper limits. As for demand D4, only the concentration of contaminant *c* needs to be checked when 6.124 t/h of source S1 is replaced by S2 at the same flow rate. Finally, the concentrations of sources S3 and S4 should be updated after breaking loop 1. From the resulting network described in Table 4, it can be observed that the concentration of contaminant *c* at S4 (marked in red) exceeds its upper bound. Luckily, this simplified network can be made feasible by performing additional two-source shift(s).

Step 4: Perform two-source shift(s) without violating concentration constraints.

There are two candidate two-source shifts, i.e., (S1, S3, D3, D4) and (S3, S4, D4, WW), as marked by green color in Table 4. The former can be utilized to reduce the concentrations in both D4 and S4 because the contaminant concentrations of S1 are much lower than those of S3 and, in addition, there are ample rooms for the concentrations of D3 and S3 to increase. The feasibility of this shift has been verified and the resulting solution is provided in Table 5.

On the other hand, the later candidate is infeasible because of the facts that a self-recycle loop involving D4 and S4 will form after the shift and, if this loop is removed, the concentration of contaminant *c* in source S4 will reach 913.25 ppm (which is obviously larger than the maximum allowed concentration of 900 ppm). Finally, since there are no other loop-breaking and source-shifting candidates, path relaxation should be considered next.

Step 5: Relax freshwater usage along one or more path.

This step is omitted because there are no candidate paths. Thus, the solution in Table 5 should be our final design.

3.2. *Example 2*

Let us consider the refinery example presented in Wang and Smith (1994), Doyle and Smith (1997) and also Li and Chang (2007). The process data for this problem can be found in Table 6. It is assumed that there are only one external source and one external sink. A reported optimal solution (Li and Chang, 2007) is adopted as the preliminary network (see Table 7). Notice that this design features a freshwater consumption level of 105.604 t/h and 9

Table 5
Evolved network after two-source shift of Example 1.

{C }	F	Streams	D1 34 {0,0,0}	D2{200,100,500} 47.22 {0,0,0}	D3{600,850,390} 16.218 {160, 450, 30}	D4{300,460,400} 65.0 {159.1, 319.2, 285.1}	WW 81.22
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S1			16.218	17.782	
{158.8,270.0,381.2}	47.22	S2				47.222	
{949.2,1128.3,1498.0}	16.218	S3					16.218
{774.3,897.4,900}	65.0	S4					65.0

Table 6
Process limiting data of Example 2.

Unit no.	Unit	Limiting F (t/h)	Contaminant	$\overline{C}^{in}_{u,k}$ (ppm)	$\overline{C}^{out}_{u,k}$ (ppm)
1	Distillation	45	Hydrocarbon	0	15
			H_2S	0	400
			Salt	0	35
2	Hydrodesulfurization	34	Hydrocarbon	20	120
			H_2S	300	12,500
			Salt	45	180
3	Desalter	56	Hydrocarbon	120	220
			H_2S	20	45
			Salt	200	9500

Table 7
Matching matrix of Example 2.

{C }	F	Streams	D1 45{0,0,0}	D2{20,300,45} 34{11.45,300,45}	D3{120,20,200} 54.831{0.73,19.47,1.70}	WW 105.604{91.62,4111.63, 4990.07}
{0,0,0}	105.604	FW	45	***8.441***	***52.163***	
{15,400,35}	45	S1		***25.492***	***2.668***	***16.840***
{111.45,12500,180}	34	S2				34
{102.86,45.0,9500}	54.831	S3		***0.067***		***54.764***

Table 8
Matching matrix after path 2 relaxation of Example 2.

{C }	F	Streams	D1 45{0,0,0}	D2{20,300,45} 34{11.25,300,26.24}	D3{120,20,200} 54.831{0.73,19.47,1.70}	WW 105.671
{0,0,0}	105.671	FW	45	***8.508***	***52.163***	
{15,400,35}	45	S1		***25.492***	***2.668***	16.840
{111.25,12500,161.24}	34	S2				34
{102.86,45.0,9500}	54.831	S3				54.831

interconnections. The same evolution steps are applicable in this example and the results are summarized below:

The target of match number is

$$N_M^{Target} = N_S + N_D - 1 = 4 + 4 - 1 = 7$$

Therefore, two matches may be eliminated from the preliminary network. It can be observed from Table 7 that two loops are present. Loops 1 and 2 are marked in cyan and green respectively, while the shared element is in red. Unfortunately, there are no opportunities for loop breakage and two-source shift in this example and, therefore, path relaxation is the only viable option left. There are three paths in the preliminary network, i.e.,

(1) (FW–D2, S1–D2, S1–WW);
(2) (FW–D2, S3–D2, S3–WW);
(3) (FW–D3, S1–D3, S1–WW).

Table 9
Matching matrix after paths 2 and 3 relaxation of Example 2.

{C }	F	Streams	D1 45{0,0,0}	D2{20,300,45} 34{11.25,300,26.24}	D3{120,20,200} 54.821{0,0,0}	WW 108.329
{0,0,0}	108.329	FW	45	8.508	54.821	
{15,400,35}	45	S1		25.492		19.508
{111.25,12500,161.24}	34	S2				34
{102.15,25.54,9500}	54.821	S3				54.821

The corresponding freshwater penalties are 25.492, 0.067 and 2.668 t/h respectively. To keep the increase of freshwater usage to a minimum level, match S3–D2 is eliminated first by path 2 relaxation. It should be noted that, in this case, the actual freshwater penalty should be equal to or less than 0.067 t/h because freshwater is much cleaner than S3 and the flow rate of D2 (the inlet stream of unit 2) is allowed to be reduced. The evolved solution is given in Table 8. Note that the concentrations of demand D2 have been altered accordingly and the resulting disturbances also propagate to the downstream source S2 and demand WW. Similarly, path 3 can be relaxed by consuming an additional 2.658 t/h of freshwater. The resulting network can be found in Table 9. The total freshwater usage in this design should be increased by $0.067+2.658=2.725$ t/h (2.6%) and the number target can be reached exactly. Finally, it should be noted that path 1 relaxation may not be needed if the aforementioned freshwater penalty (25.492 t/h) is unacceptable to the designer.

4. Conclusions

A systematic evolution approach is proposed in this paper to simplify the preliminary network design of any multi-contaminant water-using system. Specifically, the desired structures can be produced with a targeting formula and three heuristic evolution strategies. The required implementation steps are illustrated with two examples. Based on these results, one can find that the proposed strategies are quite effective and, since they are applied *locally* to loops, paths and shiftable source-demand pairs, the feasibility of the proposed approach is not dependent upon the complexity and scale of the given system.

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