Evolution of Water-Using Networks with Multiple Contaminants

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A systematic procedure is outlined in this paper to evolve a preliminary water-using network into a simpler one while incurring the lowest penalty in freshwater usage. The minimum interconnection number is first targeted on the basis of graph theory and then, three effective evolution strategies are applied to achieve this goal. The proposed procedure can be easily realized with the help of Microsoft Office Excel. An example is presented to illustrate the evolution procedure and demonstrate its effectiveness.

1. Introduction

In designing a realistic water-using network, 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 manual evolution strategies based on source shift (Prakash and Shenoy, 2005a), loop breakage (Das et al., 2009) and path relaxation (Ng and Foo, 2006), while the other is essentially model based (Das et al., 2009; Faria and Bagajewicz, 2010; Li and Chang, 2011a; Poplewski et al., 2010). The former approach is adopted in present study due to its application easiness.

It should be first pointed out that the available evolution methods were primarily developed for the fixed-flowrate operations. The inlet and outlet streams of every fixed-load unit in these 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, 2005a). This treatment is fundamentally flawed since (1) the inlet and outlet flow rates 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, 2005b). 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 (Doyle and Smith, 1997; Li and Chang, 2007, 2011b), there is a definite need to develop a generalized evolution method for practical applications.

To address this need, a heuristic procedure is developed in this work to systematically evolve from a given preliminary design into one or more improved networks with fewer

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interconnections, less total throughput and near minimum freshwater usage. In addition, both fixed-load and fixedflowrate operations are considered in this procedure.

2. Heuristic Evolution Strategies

The proposed evolution procedure can be found in Figure 1, in which the main steps are described below:

2.1 Target match number

The minimum number of interconnections must be first established as a design target. As pointed out by Prakash and Sheney (2005a), any water-using network can be characterized by a bipartite graph with nodes denoting the water streams (sources and demands) and edges denoting the

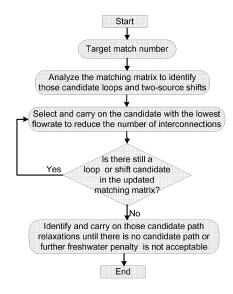


Fig. 1: Generalized evolution procedure

matches. The number of matches $(N_{\rm M})$ can then be calculated according to Euler's network theorem:

$$N_M^{bet} = N_S + N_D + N_{LP} - N_{ST} (1)$$

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 can be found in Prakash and Shenoy (2005a). It should be noted that equation (1) is applicable for any network which contains the fixed-flowrate and/or fixed-load units. Also note 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

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

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

2.2 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 constraints 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.

2.3 Two-source shift

A candidate of two-source shift can be identified according to two criteria, i.e., (1) two demands are satisfied by two different sources and only one entry is missing in the corresponding positions in matching matrix (Prakash and Shenoy, 2005a); (2) a fixed-load operation is involved in the shift and its outlet concentrations do not reach their maximums. The shift is feasible if (a) 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 (b) 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 example.

2.4 Path relaxation

A path is a series of connected matches, which starts and ends at the 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 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 example in the subsequent section.

Note that, since only this strategy 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. An Example

The process limiting data of this example are adopted from Doyle and Smith (1997) (see Table 1). Four fixed-load operations and three contaminants are present in this system. Only one external source (without contaminants) and one external demand (without any inlet concentration limit) are available. The minimum freshwater consumption rate was found to be 81.22 t/h (Doyle and Smith, 1997). An optimal solution generated by the model-based method (Li and Chang, 2007) is given in Table 2 with *matching matrix*. This solution is adopted here as the preliminary network.

Table 1: Process limiting data of example problem

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

	THE THE PERSON OF THE PERSON O	Streams	D1	D2	D3	D4	WW
{C}	F		34	47.22	20	69.63	81.22
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S1			5.982	28.018	
{158.8,270.0,381.2}	47.22	S2			9.458	37.765	
<i>{940.1,1023,</i> 1580 <i>}</i>	20	S3				3.85	16.15
{777.0,924.0,880.6}	69.63	S4			4.56		65.07

Following is a summary of the heuristic evolution steps:

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

This target is: $N_M^{bet} = N_S + N_D - 1 = 5 + 5 - 1 = 9$, 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.

The rows and columns of this matrix in Table 2 are associated with sources (FW, S1-S4) and demands (D1-D4 and WW) respectively, The actual concentrations of sources are given in italic number if they are less than their maximum values and in both **bold** and italic ones if they are larger than their maximum values. Here, D1 and S1 represent the inlet and outlet stream of unit 1 separately, and similar notations are adopted for other units. Such conventions are adopted throughout this paper. It can be observed that two independent loops and two subsets are present. Specifically, these loops are Loop 1 (S1-D3, S1-D4, S2-D4, S2-D3) and Loop 2 (S2-D3, S2-D4, S3-D4, S3-WW, S4-WW, S4-D3); and the subsets are (FW, D1, D2) and (S1, S2, S3, S4, D3, D4, WW).

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

It should be noted first that the aforementioned loops in Table 2 cannot be broken due to the concentration limits at demand D3.

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

There are three shift candidates, i.e. Shift 1 (S1, S4, D3, D4), Shift 2 (S2, S4, D3, D4) and Shift 3 (S3, S4, D4, WW). The first shift is arbitrarily performed first and the

resulting network is presented in Table 3. It should be noted that the same solution can be obtained if the second candidate is selected first while only an inferior one can be reached with the third candidate.

It can be observed from Table 3 that, although the affected concentrations of source S4 are higher than their maximum allowable values, two newly-formed source-shift candidates, i.e., (S1, S3, D3, D4) and (S2, S3, D3, D4), may be utilized to bring down these concentrations. Since both options will end up with the same final solution, the latter is adopted here for illustration convenience. The evolved network is shown in Table 4, in which another concentration violation shows up in source S3 while the previous violation in source S4 disappears.

Notice that the aforementioned Loop 1 is a breakable candidate at this point. The network in Table 4 can be made feasible by performing the corresponding loop breakage. The resulting design is given in Table 5.

Table 3: Matching matrix after two-source shift

		Streams	D1	D2	D3	D4	WW
{C}	F		34	47.22	20	65.07	81.22
{0,0,0}	81.22	FW	34	47.22			-
{160,450,30}	34	S1			10.542	23.458	
{158.8,270.0,381.2}	47.22	S2			9.458	37.765	
{799.4,914.8,1386.1}	20	S3				3.85	16.15
<i>{811.9,950.9,928.8}</i>	65.07	S4					65.07

Table 4: Matching matrix after another two-source shift

		Streams	D1	D2	D3	D4	WW
{C}	F		34	47.22	16.15	65.07	81.22
{0,0,0}	81.22	FW	34	47.22		000000000000000000000000000000000000000	000100000000000000000000000000000000000
{160,450,30}	34	S 1			10.542	23.458	
{158.8,270.0,381.2}	47.22	S2			5.608	41.615	
{952.2,1068.6, 1625.6 }	16.15	S3					16.15
{774.0,912.7,869.3}	65.07	S4					65.07

Table 5: Matching matrix after loop breakage

		Streams	D1	D2	D3	D4	WW
{C}	F		34	47.22	16.15	65.07	81.22
{0,0,0}	81.22	FW	34	47.22			
{160,450,30}	34	S 1			16.15	17.85	
{158.8,270.0,381.2}	47.22	S2				47.22	
{952.2,1131.1,1503.7}	16.15	S3					16.15
{773.9,897.2,889.6}	65.07	S4					65.07

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. Note that the number of matches in Table 5 is 7, i.e., two fewer than the target value. This is because there are three subsets in the final design.

4. Conclusions

A systematic evolution procedure is proposed in this paper to simplify the network structure of any water-using system based on a preliminary design. The implementation steps of this approach are illustrated with an example. Based on the results obtained so far, one can conclude that the proposed evolution procedure can be followed to effectively simplify the network structure of any multi-contaminant water-using system. Since the proposed heuristic strategies are applied locally to loops, paths and shiftable source-demand pairs, their feasibility is not dependent upon the complexity and scale of the given system. When compared with the model-based methods, the proposed evolution procedure can be considered as an alternative design approach to approximately optimize the water-using networks for realistic applications.

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References

- Das A. K., Shenoy U. V. and Bandyopadhyay S., 2009, Evolution of resource allocation networks. Ind. Eng. Chem. Res. 48, 7152-7167.
- Doyle S. J. and Smith R., 1997, Targeting water reuse with multiple contaminants. Trans IChemE Part B 75(Aug.), 181-189.
- Faria D. C. and Bagajewicz M. J., 2010, On the degeneracy of water/wastewater allocation problem in process plants. Ind. Eng. Chem. Res. 49, 4340-4351.
- Li B. H. and Chang C. T., 2007, A simple and efficient initialization strategy for optimizing water-using network design. Ind. Eng. Chem. Res. 46, 8781-8786.
- Li B. H. and Chang C. T., 2011a, A model-based strategy for exhaustive identification of alternative water network designs. Ind. Eng. Chem. Res. doi:10.1021/ie100310g
- Li B. H. and Chang C. T., 2011b, Heuristic evolution strategies for simplifying water-using networks with multiple contaminants. Chem. Eng. Sci. 66, 558-562.
- Ng D. K. and Foo D. C. Y., 2006, Evolution of water network using improved source shift algorithm and water path analysis. Ind. Eng. Chem. Res. 45, 8095-8104.
- Poplewski G., Walczyk K. and Jezowski J., 2010, Optimization-based method for calculating water networks with user specified characteristics. Chem. Eng. Res. Des. 88, 109-120.
- Prakash R. and Shenoy U., 2005a, Design and evolution of water networks by source shifts. Chem. Eng. Sci. 60, 2089-2093.
- Prakash R. and Shenoy U., 2005b, Targeting and design of water networks for fixed flowrate and fixed contaminant load operations. Chem. Eng. Sci. 60, 255-268.