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Multiobjective Optimization of Water-Using Networks with Multiple Contaminants

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ABSTRACT: A systematic multiobjective optimization procedure is developed in this study to produce realistic multicontaminant water-using network designs. In every given design problem, the most appropriate structure is identified by solving three mathematical programming models (that is, one nonlinear program and two mixed-integer nonlinear programs) sequentially so as to satisfy different criteria in order of decreasing importance. Freshwater conservation is given the top priority in the present work because of its scarcity in environment and the pollution problems caused by wastewater effluents. Minimization of the total number of interconnections in the water network is treated as the next design goal since network complexity is directly related to operability, controllability and safety. The final step in the sequential procedure is to minimize the total throughput and, consequently, the operating and capital costs of all water using units as well. Five examples are presented in this paper to demonstrate the effectiveness of proposed procedure. When compared with the network designs obtained with available methods reported in literature, it can be observed that better solutions can usually be generated with our approach.

1. INTRODUCTION

Industrial water network synthesis[1] 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, that is, the pinch-based[2] and the model based approaches .[3] Good reviews have been provided by Bagajewicz,[4] Foo[5] and Jezowski[6] with somewhat different emphases. For any water-using process, it is possible to identify more than one network structure that requires the minimum level of freshwater usage. Among them, the one with the fewest interconnections is usually selected because of practical considerations, such as operability, controllability, and ease of implementation.[7] Two distinct approaches have been taken to produce "simple" network configurations. One is to perform manual evolution from an existing network by using *source shift*,[8] *loop breaking*,[7] and *path relaxation*,[9] while the other is also model based .[7,10−13]

Prakash and Shenoy[8] first proposed a manual *source-shift algorithm* (SSA) to evolve from a preliminary design to network structures with fewer matches. Ng and Foo[9] later argued that the original version of source-shift strategy was iterative in nature, 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,[14] was also proposed to relax the upper bound of freshwater consumption rate so as to simplify network configuration. Recently, Das et al.[7] 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) without incurring significant penalties. It should be pointed out that the aforementioned evolution methods were mainly developed for the fixed-flow rate operations .[15] Specifically, the inlet and outlet streams of every fixed-load operation were treated as *independent* demand and source, while the material-balance relation between their flow rates was ignored.[7−9,16]

On the other hand, the model-based method was traditionally applied to generate the optimal designs based on one objective function, for example, the total annual cost (TAC). Since it is often more realistic to evaluate the performance of a water network with several different economic and also noneconomic criteria, a number of sequential optimization strategies have been developed in recent years. By and large, the available sequential approaches are limited to water-using processes with only a single key contaminant or only the fixed-flow rate operations.[10,11,13,15] This is mainly because all model constraints are linear in these situations. In particular, a linear program (LP) can be first adopted to minimize the freshwater usage and a mixed-integer linear program (MILP) can then be used to minimize the total interconnection number while keeping the freshwater consumption level at its minimum .[10,11] Another MILP model can be solved[13] at last to minimize the total throughput of fixed load operations[15] under the constraints of fixed freshwater consumption rate and interconnection number. Since multiple contaminants are present in almost all industrial water networks,[1,17,18] it is obviously necessary to generalize the sequential optimization approach to the multicontaminant systems.

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For this purpose, a series of three mathematical programming models are proposed in this work to address three different design issues sequentially. Freshwater conservation is given the top priority in the present work because of its scarcity in environment and the pollution problems caused by wastewater effluents. Minimization of the total number of interconnections in the water network is treated as the next design goal since network complexity is directly related to operability, controllability and safety. The final step in the sequential procedure is to minimize the total throughput and, consequently, the operating and capital costs of all water using units as well. More specifically, these different optimization tasks are accomplished in this study with the following strategies:

1. A nonlinear programming (NLP) model is formulated to find the minimum level of freshwater consumption rate. The initialization strategy developed by Li and Chang[17] can be used to generate a good initial guess.
2. A mixed-integer nonlinear programming (MINLP) model is constructed to minimize the interconnection number while keeping the freshwater usage at its minimum or a slightly relaxed level. The solution of the aforementioned NLP model can be used as the initial guess.
3. Another MINLP model is built to minimize the total throughput of fixed-load operations under the constraints of assigned freshwater consumption rate and interconnection number. The optimization results obtained in solving the above MINLP model can be used as a feasible initial guess.

Finally, it should be noted that both fixed-load and fixed-flow rate operations can be considered in all models mentioned above.

This paper is structured as follows. A formal problem statement is first provided in the next section. The general model constraints are presented in section 3, and the model solution strategy is outlined next in section 4. The effectiveness of the proposed optimization strategy is clearly demonstrated in all five examples. Finally, specific conclusions are given at the end of this paper.

2. PROBLEM STATEMENT

To generate a desired water-using network design, it is assumed that the following process data are available:

- a set of contaminants
- a set of fixed-load operations and each is specified by
  - its contaminant load to be removed
  - the maximum inlet and outlet concentrations
  - water loss or gain during operation
- a set of *internal* water sources or sinks/demands (i.e., the fixed-flow rate operations) and each is specified by
  - its water flow rate and contaminant concentrations in the former case
  - its water flow rate and upper bounds of contaminant concentrations in the latter case
- a set of *external* water sources and each is specified by
  - its contaminant concentrations
  - the maximum supply rate
- a set of *external* sinks/demands and each is specified by
  - the upper limit of water flow rate
  - the maximum inlet contaminant concentrations

On the basis of these process data, it is the goal of the present design task to identify a network configuration by sequentially striving for (1) the lowest freshwater usage, (2) the smallest total number of interconnections, and (3) the minimum total throughput.

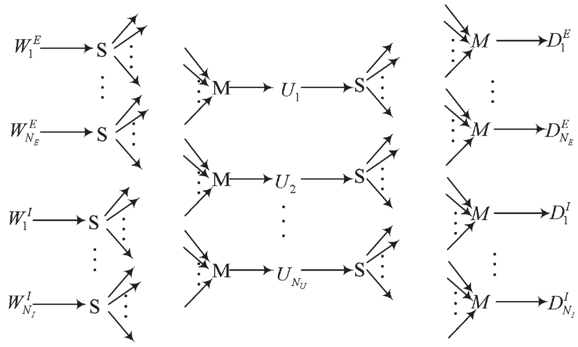

Figure 1. General superstructure of water-using network.

3. GENERAL MODEL CONSTRAINTS

3.1. Superstructure. To develop a general model formulation, it is necessary to first build a superstructure in which all possible flow connections are embedded. Although the superstructure presented here is the same as that given in Li and Chang,[13] a brief description is still provided for the sake of completeness. Specifically, a unique label is assigned to each source, each demand and every fixed-load unit and these labels are collected in the following sets:

$$\mathbb{W} = \{w | w \text{ is the label of a water source}\} \quad (1)$$

$$\mathbb{D} = \{d | d \text{ is the label of a water demand}\} \quad (2)$$

$$\mathbb{U} = \{u | u \text{ is the label of a fixed-load unit}\} \quad (3)$$

Notice that,

$$\mathbb{W} = \mathbb{W}_1 \cup \mathbb{W}_2$$

and

$$\mathbb{W}_1 = \{w_1 | w_1 \text{ is the label of an external source}\} \quad (4)$$

$$\mathbb{W}_2 = \{w_2 | w_2 \text{ is the label of an internal source}\} \quad (5)$$

Similarly,

$$\mathbb{D} = \mathbb{D}_1 \cup \mathbb{D}_2$$

and

$$\mathbb{D}_1 = \{d_1 | d_1 \text{ is the label of an external demand}\} \quad (6)$$

$$\mathbb{D}_2 = \{d_2 | d_2 \text{ is the label of an internal demand}\} \quad (7)$$

On the basis of the above set definitions, a superstructure can be constructed according to Figure 1, in which the symbols S and M denote the splitting and mixing node, respectively.[13]

3.2. Model Constraints. The following model constraints can then be formulated on the basis of superstructure:

3.2.1. At the Splitting Nodes after the Water Sources. The water balances can be expressed as

$$sr_w = \sum_{u \in \mathbb{U}} f_{w,u}^W + \sum_{d \in \mathbb{D}_w} f_{w,d}^W \quad w \in \mathbb{W} \quad (8)$$

where sr_w is the water supply rate from source w; $f_{w,u}^W$ and $f_{w,d}^W$ denote the flow rates of waters (from source w) which are consumed by unit u and demand d respectively; $\mathbb{D}_w$ is a set defined as

$$\mathbb{D}_w = \begin{cases} \mathbb{D}_2 & \text{if } w \in \mathbb{W}_1 \\ \mathbb{D} & \text{if } w \in \mathbb{W}_2 \end{cases} \quad (9)$$

The supply limit of the external sources can be expressed as

$$sr_w \leq S_w \quad w \in \mathbb{W}_1 \quad (10)$$

And the internal waters must be completely consumed, and their supply rates are assumed to be constants in this study; the following constraints should also be imposed:

$$sr_w = S_w \quad w \in \mathbb{W}_2 \quad (11)$$

where S_w is a given design parameter.

3.2.2. At the Splitting Nodes after the Fixed-Load Units. The water balance at the splitting node after fixed-load unit u can be written as

$$f_u^{out} = \sum_{u' \in \mathbb{U}, u' \neq u} f_{u,u'} + \sum_{d \in \mathbb{D}} f_{u,d}^D \quad u \in \mathbb{U} \quad (12)$$

where, f_u^{out} is the water flow rate at the outlet of unit u; $f_{u,u'}$ represents the water flow rate from unit u to unit u'; $f_{u,d}^D$ is the flow rate of wastewater generated by unit u and sent to demand d.

The upper limit of the outlet concentration of each unit can be expressed as

$$c_{u,k}^{out} \leq \overline{C}_{u,k}^{out} \quad u \in \mathbb{U} \quad k \in \mathbb{K} \quad (13)$$

where, $\mathbb{K}$ is the set of all possible contaminants, $c_{u,k}^{out}$ denotes the concentration of contaminant k at the outlet of unit u, and $\overline{C}_{u,k}^{out}$ represents the corresponding upper bound (which is a given parameter).

3.2.3. At the Mixing Nodes before the Fixed-Load Units. The water balance around the mixing node can be written as

$$f_u^{in} = \sum_{u' \in \mathbb{U}, u' \neq u} f_{u',u} + \sum_{w \in \mathbb{W}} f_{w,u}^W \quad u \in \mathbb{U} \quad (14)$$

where f_u^{in} is the total flow rate at the mixing node of unit u; $f_{u',u}$ is the water flow rate from unit u' to unit u. The corresponding mass balance of contaminant should be

$$f_u^{in} c_{u,k}^{in} = \sum_{u' \in \mathbb{U}, u' \neq u} f_{u',u} c_{u',k}^{out} + \sum_{w \in \mathbb{W}} f_{w,u}^W C_{w,k} \quad u \in \mathbb{U} \quad k \in \mathbb{K} \quad (15)$$

where $c_{u,k}^{in}$ denote the concentration of contaminant k at the inlet of unit u; $C_{w,k}$ denotes the concentration of contaminant k from water source w, which is a given parameter.

Finally, a upper bound ($\overline{C}_{u,k}^{in}$) must be imposed upon the inlet concentration of each fixed-load unit, i.e.

$$c_{u,k}^{in} \leq \overline{C}_{u,k}^{in} \quad u \in \mathbb{U} \quad k \in \mathbb{K} \quad (16)$$

3.2.4. At the Mixing Nodes before the Water Demands. The water and contaminant balances are

$$f_d^{in} = \sum_{u \in \mathbb{U}} f_{u,d}^D + \sum_{w \in \mathbb{W}_d} f_{w,d}^W \quad d \in \mathbb{D} \quad (17)$$

$$f_d^{in} \overline{C}_{d,k}^{in} \geq \sum_{u \in \mathbb{U}} f_{u,d}^D c_{u,k}^{out} + \sum_{w \in \mathbb{W}_d} f_{w,d}^W C_{w,k} \quad d \in \mathbb{D} \quad k \in \mathbb{K} \quad (18)$$

where f_d^{in} is the total water flow rate delivered to demand d; $\overline{C}_{d,k}^{in}$ is the maximum concentration of contaminant k allowed at sink d; the set $\mathbb{W}_d$ is defined as

$$\mathbb{W}_d = \begin{cases} \mathbb{W}_2 & \text{if } d \in \mathbb{D}_1 \\ \mathbb{W} & \text{if } d \in \mathbb{D}_2 \end{cases} \quad (19)$$

For each internal demand, the flow-rate requirement must be strictly satisfied, that is,

$$f_d^{in} = F_d^D \quad d \in \mathbb{D}_2 \quad (20)$$

where F_d^D is required flow rate by demand d.

3.2.5. Performance Models of the Fixed-Load Units. The process performance of fixed-load unit u can be characterized as

$$f_u^{in} = f_u^{out} + F_u^L \quad u \in \mathbb{U} \quad (21)$$

$$f_u^{in} c_{u,k}^{in} + M_{u,k} = f_u^{out} c_{u,k}^{out} + F_u^L C_{u,k}^L \quad u \in \mathbb{U} \quad k \in \mathbb{K} \quad (22)$$

where, F_u^L are the flow rate loss of unit u, $C_{u,k}^L$ is the concentration of contaminant k in the loss stream, and $M_{u,k}$ denotes the mass load of contaminant k in unit u. Notice that they are all given parameters.

To avoid redundant reuse or recycle streams around any fixed-load unit, the following constraints are imposed:

$$f_u^{in} \leq F_u^{lim} \quad u \in \mathbb{U} \quad (23)$$

where F_u^{lim} is the limiting flow rate of unit u, which can be calculated with the following formulas:

$$F_u^{lim} = \max_k G_{u,k}^{lim} \quad u \in \mathbb{U} \quad (24)$$

and

$$G_{u,k}^{lim} = (M_{u,k} - F_{u,k}^L C_{u,k}^L)/(\overline{C}_{u,k}^{out} - \overline{C}_{u,k}^{in}) \quad u \in \mathbb{U} \quad k \in \mathbb{K} \quad (25)$$

Table 1. Process Limiting Data of Example 1

unit no.	unit	limiting F (t/h)	contaminant	$\overline{C}_{u,k}^{in}$ (ppm)	$\overline{C}_{u,k}^{out}$ (ppm)
1	distillation	45	hydrocarbon	0	15
			H_2S	0	400
			salt	0	35
2	hydrodesulfurization	34	hydrocarbon	20	120
			H_2S	300	12500
			salt	45	180
3	desalter	56	hydrocarbon	120	220
			H_2S	20	45
			salt	200	9500

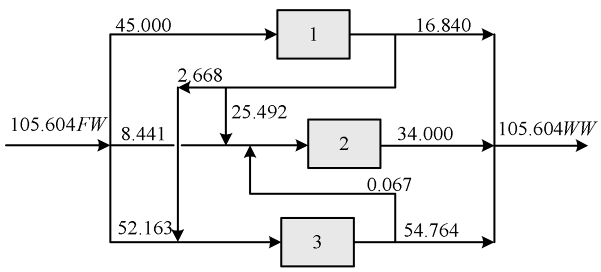

Figure 2. Preliminary network of Example 1.

Table 2. Matching Matrix of Example 1

			D1	D2{20,300,45}	D3{120,20,200}	WW
{C}	F	streams	45{0,0,0}	34{**11.45**,300,45}	54.831{**0.73,19.47,1.70**}	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 3. Matching Matrix after Relaxing Freshwater Usage by 0.067 t/h in Example 1

			D1	D2{20,300,45}	D3{120,20,200}	WW
{C}	F	streams	45{0,0,0}	34{**11.25**,300,**26.24**}	54.831{**0.73,19.47,1.70**}	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

Table 4. Matching Matrix after Relaxing Freshwater Usage by 2.735 t/h in Example 1

			D1	D2{20,300,45}	D3{120,20,200}	WW
{C}	F	streams	45{0,0,0}	34{**11.25**,300,**26.24**}	54.821{**0,0,0**}	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

Table 5. Comparison of the Optimal Network Obtained by Different Methods for Example 1

method	objective	freshwater usage (t/h)	no. of matches	min flow rate of stream (t/h)	total throughput (t/h)
targeting method[22]	Min FW	105.59	9	0.067	133.83
targeting method[22]	Min FW + forbidden reuse	105.67	8	2.668	133.83
NLP method[17]	Min FW	105.604	9	0.067	133.82
heuristic method[24]	unclear	105.65	8	2.668	135.0
sequential models	Min tn under TP = 0	105.60	9	0.067	133.82
sequential models	Min tn under TP = 0.067	105.67	8	2.668	133.83
sequential models	Min tn under TP = 2.735	108.33	7	8.508	133.82

It is obvious that $G_{u,k}^{\lim}$ denotes the limiting flow rate required by contaminant k in unit u.

It should be noted that, because of the bilinear items in constraints 15, 18, and 22, the mathematical programming models considered in this work should be NLP or MINLP.

4. SOLUTION STRATEGY

As mentioned previously, three distinct optimization steps are performed sequentially in this study for the purpose of generating a realistic configuration with NLP and MINLP models. To identify a near-optimum solution for each model, a dedicated initialization strategy has been developed and the various different solvers available in GAMS environment[19] (including BARON[20]) have all been tried. The best solution obtained in each step is kept for use in the next step. It should be pointed out that, according to our experience in solving the above-mentioned models, the optimal solutions (*even* the integer values) usually can not be obtained without proper initial guesses. Finally, notice that a thorough discussion on the global optimization strategies for various

Table 6. Process Limiting Data of Example 2

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
		a	300	800
4	80	b	460	930
		c	400	900

Table 7. Optimal Network for Example 2

			D1	D2{200,100,500}	D3{600,850,390}	D4{300,460,400}	WW
			34	47.222	16.184	65.038	81.222
{C}	F	streams	{0,0,0}	**{0,0,0}**	**{160, 450, 30}**	**{159.1, 319.3, 285.0}**	
{0,0,0}	81.222	FW	34	47.222			
{160,450,30}	34	S1			16.184	17.816	
{158.8,270.0,381.2}	47.222	S2				47.222	
{950.9,1129.7,1500.6}	16.218	S3					16.184
{774.3,897.4,900}	65.038	S4					65.038

Table 8. Comparison of the Optimal Network Obtained by Different Methods for Example 2

method	objective	freshwater usage (t/h)	no. of matches	Min flow rate of stream (t/h)	total throughput (t/h)
targeting method[22]	Min FW	81.22	N/A	N/A	N/A
heuristic method[24]	unclear	81.22	8	0.82	161.58
sequential models	Min tn under TP = 0	81.22	7	16.184	162.44

water-network synthesis problems can be found in Karuppiah and Grossmann.[21]

A summary of the proposed sequential search procedure is given below.

4.1. Determine the Minimum Freshwater Consumption Rate with a NLP Model. The objective function of the proposed NLP model can be expressed as

$$\min \quad \mathrm{tc} = \sum_{w \in \mathbb{W}_1} sr_w$$

where tc denotes the total freshwater consumption rate. Notice that eqs 8 - 23 are used as the constraints of this NLP model. The resulting minimum value of tc (denoted as $\underline{\mathrm{TC}}$) is used as a constant in the subsequent model. The initialization strategy developed by Li and Chang[17] is adopted in this work to generate a near-feasible initial guess to facilitate convergence.

4.2. Determine the Minimum Interconnection Number with a MINLP Model. The objective function in this case is

$$\min \quad \mathrm{tn} = \sum_{w \in \mathbb{W}} \sum_{u \in \mathbb{U}} n^W_{w,u} + \sum_{w \in \mathbb{W}} \sum_{d \in \mathbb{D}} n^W_{w,d} + \sum_{u' \in \mathbb{U}} \sum_{u \in \mathbb{U}} n_{u',u} + \sum_{u \in \mathbb{U}} \sum_{d \in \mathbb{D}} n^D_{u,d}$$

where $n^W_{w,u}$, $n^W_{w,d}$, $n_{u',u}$, and $n^D_{u,d}$ are binary variables and each is used to reflect whether or not the corresponding branch stream exists. In particular, they are constrained in the proposed model with the following inequalities:

$$f^W_{w,u} \le n^W_{w,u} S_w \quad f^W_{w,d} \le n^W_{w,d} S_w \quad w \in \mathbb{W} \quad u \in \mathbb{U} \quad d \in \mathbb{D} \tag{26}$$

$$f_{u',u} \le n_{u',u} F^{\lim}_{u'} \quad f^D_{u,d} \le n^D_{u,d} F^{\lim}_{u} \quad u, u' \in \mathbb{U} \quad d \in \mathbb{D} \tag{27}$$

The following inequality constraint is also needed to keep the total freshwater consumption rate below an acceptable level:

$$\underline{\mathrm{TC}} + \mathrm{TP} \ge \sum_{w \in \mathbb{W}_1} sr_w \tag{28}$$

where TP ≥ 0 is a user-selected relaxation parameter. The main purpose for introducing the relaxation parameter TP in eq 28 is to remove the branch streams with extremely small flow rates. In actual optimization run, this parameter should be set to be the sum of these negligible flow rates. Obviously, TP provides the flexibility for designer to simplify the water-using network under his/her control.

Table 9. Process Data of Example 3

unit no.	contaminant	load (kg/h)	$\overline{C}^{in}_{u,k}$ (ppm)	$\overline{C}^{out}_{u,k}$ (ppm)
1	A	3.40	20	120
	B	414.80	300	12500
	C	4.59	45	180
2	A	5.60	120	220
	B	1.40	20	1000
	C	520.80	200	9500
3	A	0.16	0	20
	B	0.48	0	60
	C	0.16	0	20
4	A	0.80	50	150
	B	60.80	400	8000
	C	0.48	60	120
5	A	0.75	0	15
	B	20.00	0	400
	C	1.75	0	35
6	A	2.00	10	70
	B	100.70	200	600
	C	2.50	20	90
7	A	1.80	25	150
	B	6.80	230	1000
	C	0.60	20	220
8	A	3.00	5	100
	B	102.30	45	4000
	C	8.14	50	300
9	A	4.60	13	100
	B	200.00	200	3000
	C	1.90	5	200
10	A	4.00	10	100
	B	10.30	90	500
	C	9.0	70	800

In summary, the constraints of the present MINLP model should include eqs 26−28 and all those in the previous NLP model. The minimum objective value of this model is referred to as $\underline{\mathrm{TN}}$, and this value is adopted as a constant in the third model. The initial guesses of the continuous variables in this MINLP

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model can be obtained from the optimal solution of the previous NLP model. As for the binary variables, the following initialization steps should be applied:

$$(n_{w,u}^{W}).l = 1 \text{ if } (f_{w,u}^{W}).l \geq \epsilon \quad w \in \mathbb{W} \quad u \in \mathbb{U}$$

$$(n_{w,d}^{W}).l = 1 \text{ if } (f_{w,d}^{W}).l \geq \epsilon \quad w \in \mathbb{W} \quad d \in \mathbb{D}$$

$$(n_{u',u}).l = 1 \text{ if } (f_{u',u}).l \geq \epsilon \quad u, u' \in \mathbb{U}$$

$$(n_{u,d}^{D}).l = 1 \text{ if } (f_{u,d}^{D}).l \geq \epsilon \quad u \in \mathbb{U} \quad d \in \mathbb{D}$$

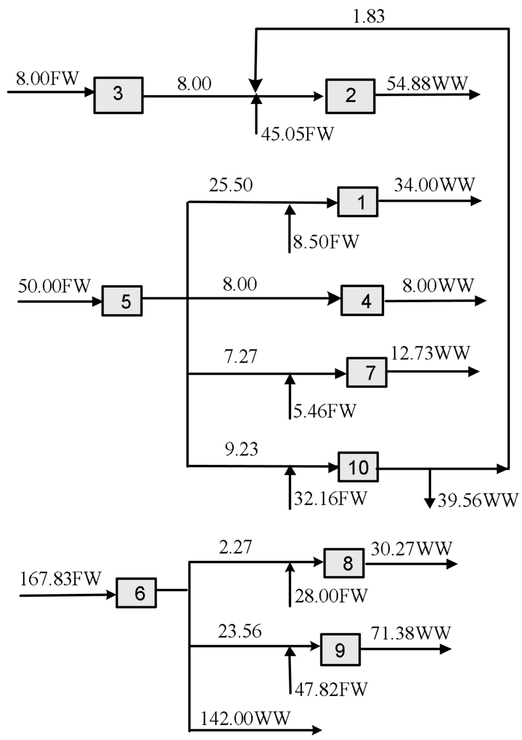

Figure 3. Optimal solution of Example 3.

where ϵ is a small positive number to account for the truncation errors, and $(f_{w,u}^{W}).l$ denotes the initial guess and also optimal value of $f_{w,u}^{W}$ (obtained from the solution of NLP model). Notice that the other symbols can be interpreted with the same principle. After solving this model, the actual freshwater consumption rate $\underline{\text{TC}}_{\text{relax}}$ can be calculated by

$$\underline{\text{TC}}_{\text{relax}} = \sum_{w \in \mathbb{W}_1} (sr_w).l$$

in which $(sr_w).l$ is the optimal value of (sr_w) obtained from the solution of the present MINLP model.

4.3. Determine the Minimum Total Throughput with Another MINLP Model. It should be noted first that this model can be neglected if no fixed-load operations are present in the network. Since the input or output flow rate of every fixed-flow rate operation must be kept unchanged, the total throughput of a water network can be minimized by minimizing that of all fixed-load units. Thus, the objective function of this model can be written as

$$\min \quad \text{tt} = \sum_{u \in \mathbb{U}} f_u^{\text{in}}$$

where tt is the total throughput of all fixed-load operations. The following constraints are introduced in the present model to impose upper bounds on the total connection number and the water consumption rate respectively:

$$\underline{\text{TN}} \geq \sum_{w \in \mathbb{W}} \sum_{u \in \mathbb{U}} n_{w,u}^{W} + \sum_{w \in \mathbb{W}} \sum_{d \in \mathbb{D}} n_{w,d}^{W} + \sum_{u' \in \mathbb{U}} \sum_{u \in \mathbb{U}} n_{u',u} + \sum_{u \in \mathbb{U}} \sum_{d \in \mathbb{D}} n_{u,d}^{D} \tag{29}$$

$$\underline{\text{TC}}_{\text{relax}} \geq \sum_{w \in \mathbb{W}_1} sr_w \tag{30}$$

Thus, the model constraints in this case are eqs 26, 27, 29, and 30, and all those in the aforementioned NLP model. The optimal solution of previous MINLP model can be used directly as the initial guess for the present model without any additional initialization step.

Table 10. Matching Matrix of Optimal Solution for Example 3

		D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	WW
F	streams	34.00	54.88	8.00	8.00	50.00	167.83	12.73	30.27	71.38	41.38	
392.82	FW	8.50	45.05	8.00		50.00	167.83	5.46	28.00	47.82	32.16	
34.00	S1											34.00
54.88	S2											54.88
8.00	S3		8.00									
8.00	S4											8.00
50.00	S5	25.50			8.00			7.27			9.23	
167.83	S6								2.27	23.56		142.00
12.73	S7											12.73
30.27	S8											30.27
71.38	S9											71.38
41.38	S10		1.83									39.56

Table 11. Comparison of the Optimal Network Obtained by Different Methods for Example 3

method	objective	freshwater usage (t/h)	no. of matches	Min flow rate of stream (t/h)	total throughput(t/h)
MINLP model[17]	Min FW under struct. cons	392.816	27	1.0	478.86
Sequential models	Min tn under TP=1.967	392.816	25	1.827	478.48

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Table 12. Process Data of Example 4

unit no.	limiting Flow rate (t/h)	contaminant	$\overline{C}^{in}_{u,k}$ (ppm)	$\overline{C}^{out}_{u,k}$ (ppm)
1	30	A	0	100
		B	0	90
		C	0	50
2	16	A	0	50
		B	0	70
		C	0	70
3	75	A	40	150
		B	60	80
		C	20	70
4	21	A	30	160
		B	40	100
		C	70	90
5	29	A	110	210
		B	135	200
		C	60	120
6	40	A	200	350
		B	170	400
		C	150	210
7	61	A	100	300
		B	75	290
		C	20	170
8	57	A	90	210
		B	50	170
		C	34	100

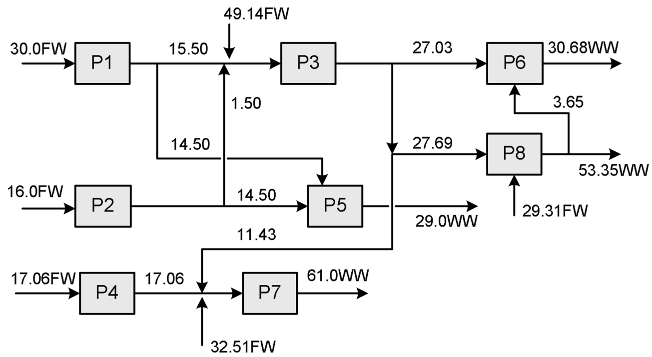

Figure 4. Optimal solution of Example 4.

Table 13. Matching Matrix of Optimal Solution for Example 4

		D1	D2	D3	D4	D5	D6	D7	D8	WW
F	streams	30.00	16.00	66.14	17.06	29.00	30.68	61.00	57.00	174.03
174.03	FW	30.00	16.00	49.14	17.06			32.51	29.31	
30.00	S1			15.50		14.50				
16.00	S2			1.50		14.50				
49.14	S3						27.03	11.43	27.69	
17.06	S4							17.06		
29.00	S5									29.00
30.68	S6									30.68
61.00	S7									61.00
57.00	S8						3.65			53.35

Table 14. Comparison of the Optimal Network Obtained by Different Methods for Example 4

method	objective	freshwater usage (t/h)	no. of matches	min flow rate of stream (t/h)	total throughput (t/h)
Heuristic design[24]	unclear	174.95	20	2.81	319.83
Sequential models	Min tn under TP=0	174.03	19	1.5	306.89

5. APPLICATIONS

Five examples are presented here to demonstrate the effectiveness of the proposed sequential optimization strategy. All models were solved within the GAMS environment (version 23.3.3)[19] on a PC with an Intel(R) Core(TM) CPU at 2.66 GHz. MINOS or CONOPT was adopted for solving the NLP model. CPLEX[20] was used to solve the mixed-integer programming (MIP) models (required by the MINLP solver), while BARON, DICOPT, or SBB[20] was utilized to perform the optimization runs needed for the proposed MINLP models.

5.1. Example 1. Let us first consider the process data given in Table 1, which is a simplified version extracted from a petroleum refining process. This example was originally studied by Wang and Smith,[2] and later redesigned by Doyle and Smith,[22] Li and Chang,[17] and also Liu et al. .[24] It is assumed that there are only one freshwater source (in which all contaminant concentrations are 0 ppm) and one wastewater sink (which is without any upper contaminant concentration limit).

A reported optimal solution[17] is shown in Figure 2. Notice that the freshwater consumption rate required in this design is 105.604 t/h and there are 9 interconnections. Table 2 is the corresponding matching matrix .[7,8] Note that the inlet and outlet stream of Unit 1 is treated as demand D1 and source S1 respectively in this table and similar treatment can also be found for other units. The rows and columns of the *matching matrix* are associated with sources (FW, S1−S3) and demands (D1−D3 and WW) respectively, while their process data are given in the cells in the far-left columns 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. The first row of this matching matrix represents a freshwater (FW) source, whereas the last column is the wastewater (WW). The actual demand concentrations are given in boldfaced numbers if they are less than their maximum values. The same conventions are adopted throughout this paper.

The proposed sequential optimization procedure has been applied to the present example. Solver CONOPT was selected for the NLP model and solver BARON for the MINLP ones .[20] It was found that the CPU time was less than 0.1 s in all optimization runs. The obtained results can be summarized as follows:

1. A total of 40 continuous variables and 31 constraints were included in the NLP model, while there were 15 binary variables, 40 continuous variables and 47 constraints in the first MINLP problem. From the NLP solution, the minimum freshwater consumption rate was also found to be 105.604 t/h. By setting TP to be zero, the minimum

Table 15. Process Data of Example 5

process	contaminant	load (kg/h)	$\overline{C}_{u,k}^{m}$ (ppm)	$\overline{C}_{u,k}^{out}$ (ppm)
CDU	HC	0.675	0	15
	H_2S	18.0	0	400
	salts	1.575	0	35
HDS	HC	3.4	20	120
	H_2S	414.8	300	12500
	salts	4.59	45	180
Desalter	HC	0.801	120	220
	H_2S	0.200	20	45
	salts	000.0	200	125000
Others	HC	0.418	0	22
	H_2S	2.280	0	120
	salts	0.570	0	30
CT	HC	9.75	150	225
	H_2S	1.30	200	310
	salts	13.0	250	350
Boiler	HC	0	0	0
	H_2S	0	0	0
	salts	340	0	2000
Coker	HC	4.93	100	270
	H_2S	100.92	20	3500
	salts	5.80	50	250

number of interconnections (i.e., 9) was determined by solving the first MINLP model. The resulting network is the same as that shown in Figure 2.

2. Since match S3-D2 has the minimum flow rate of 0.067 t/h in Figure 2, TP was set at this value in the second optimization run of the first MINLP model. The corresponding optimal solution can be found in Table 3. Notice that this design has the same qualities as those of the reported one (by Liu et al.[24]) both in terms of the freshwater usage and the total interconnection number. Next, the value of TP was increased by an additional 2.668 t/h, which is essentially the minimum spent-water flow rate used for the matches in Table 3 (i.e., the flow rate of match S1−D3). The new optimal solution (see Table 4) can be obtained by rerunning the MINLP model for the third time. It is not surprising to find that the actual freshwater penalty of 2.725 t/h in Table 4 is less than 2.735 (= 0.067 + 2.668) t/h since inequality condition in eq 30 holds exactly.
3. The second MINLP model was then utilized to determine the minimum total throughput (133.83 t/h). Since no structural changes can be identified in the optimal solution, the final network configuration should be the same as that in Table 4.

Finally, a comparison between our results and those reported in three previous studies[17,22,24] is provided in Table 5. In this table, the abbreviated term "Min FW" represents minimum freshwater usage, "Min tn" represents minimum interconnection number and "+ forbidden reuse" represents additional constraints to forbid some reuse streams. Notice also that, since somewhat different design objectives were adopted in different studies, these objectives are explicitly given in the second column. From Table 5, it is clear that the solutions obtained with the proposed method are of the same (or slightly better) quality, and these solutions should be regarded as design alternatives which are more consistent with the desired priority set in the present study.

5.2. Example 2. The second example is obtained from Doyle and Smith[22] (see Table 6). Notice that three contaminants are present in this system, and there are four fixed-load operations, one freshwater source and one external wastewater sink (which is without any inlet concentration constraint). The minimum freshwater consumption rate was determined to be 81.22 t/h .[22]

A total of 41 constraints and 57 continuous variables are present in the NLP model, while there are 66 constraints, 24 binary and 57 continuous variables in the first MINLP model. Solver CONOPT was selected for the former model and BARON for the latter .[20] The CPU time needed for each model was less than 0.2 s. As usual, the value of *TP* was initially set to be zero. From the corresponding optimal solutions, the minimum freshwater consumption rate and the minimum number of interconnections were found to be 81.222 t/h and 7 respectively. The optimal solution of the first MINLP model is given in Table 7. Since the minimum branch-streamflow rate is 16.184 t/h in Table 7 and, thus, none of the matches are negligible, there is no need to increase the value of TP to further simplify the network. The second MINLP model was then solved to minimize the total throughput and its value was found to be 162.44 t/h. Since again no structural modifications can be identified, the network given in Table 7 should be the final design. It should be noted that, although the same freshwater consumption rates are required in both cases, the interconnection number of this network is one less than that reported in Liu et al.[24] A comparison with the published results is also summarized in Table 8.

5.3. Example 3. Let us consider a more complex system described by the process data in Table 9. In this system, there are three contaminants, ten fixed-load operations, one external source and one wastewater sink. Without any structural constraint, the minimum freshwater consumption rate was determined to be 390.849 t/h.[17] This value was later increased to 392.816 t/h by introducing additional inequalities to limit the maximum numbers of branches entering every mixing node and leaving every splitting node, and to impose upper and lower bounds of the water flow rate in each stream. The corresponding interconnection number was found to be 27 in this case.[17]

The minimum freshwater consumption rate of 390.849 t/h in the unconstrained problem can be verified with the proposed NLP model (in which there are 101 constraints and 201 continuous variables). MINOS was used for solving this NLP model and the needed CPU time was 0.1 s. By setting TP = 0, the minimum number of interconnections can be determined to be 31 with the first MINLP model (in which there are 222 constraints, 120 binary variables and 201 continuous variables). Solver DICOPT was used to perform the optimization run and the required CPU time is 0.5 s.

For comparison purpose, TP was then reset to 1.967 t/h and thus the upper limit of freshwater consumption rate was relaxed to 392.816 t/h. By rerunning the first MINLP, it was found that the minimum number of interconnections could be reduced from the reported value of 27 to 25 and the corresponding minimum branch-streamflow rate was 1.827 t/h. By solving the second MINLP model (within 18.3 s CPU time), the minimum total throughput was determined to be 478.476 t/h and the resulting optimal solution can be found in Figure 3 and also in Table 10. A comparison between the key features of the current solution and those of the reported one is provided in Table 11. From these results, it is obvious that simpler networks with insignificant penalties in freshwater usage can almost always be

Table 16. Comparison of the Optimal Network Obtained by Different Methods for Example 5

method	objective	freshwater usage (t/h)	no. of matches	min flow rate of stream (t/h)	total throughput (t/h)
MINLP model[18]	Min FW	1053.4	20	N/A	N/A
heuristic design[24]	unclear	1057.24	17	1.33	1119.78
sequential models	Min tn under TP = 0	1051.13	23	0.13	1020.68
sequential models	Min tn under TP = 2.27	1053.4	16	0.917	1020.24
sequential models	Min tn under TP = 6.11	1056.02	14	14.18	1020.02

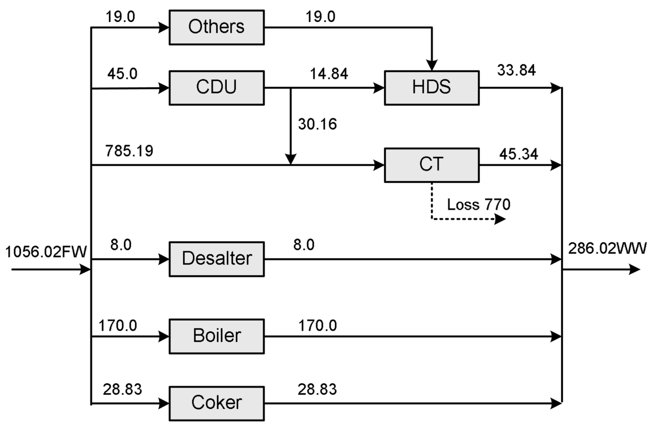

Figure 5. Optimal solution of Example 5.

Table 17. Matching Matrix of Optimal Solution for Example 5

		D1	D2	D3	D4	D5	D6	D7	WW
F	Streams	45.00	33.84	8.00	19.00	815.34	170.00	28.83	286.02
1056.02	FW	45.00		8.00	19.00	785.19	170.00	28.83	
45.00	S1		14.84			30.16			
33.84	S2								33.84
8.00	S3								8.00
19.00	S4		19.00						
45.34	S5								45.34
170.00	S6								170.00
28.83	S7								28.83

produced by following the proposed sequential optimization procedure. Notice also that the minimum branch-streamflow rate is increased from 1 t/h (which was just equal to the lower bound of water flow rate specified by the designer[17]) to 1.827 t/h without imposing any flow-rate constraint. This outcome can be attributed to the objective function of the first MINLP model.

5.4. Example 4. The original process data used in this example are taken from Wang et al.[23] (see Table 12). It is assumed that only one external source and one external sink are available here. This problem has also been studied by Liu et al.[24] using a heuristic design procedure. The reported minimum freshwater rate is 174.95 t/h and the interconnection number in optimal solution is 20.

To create a more realistic design with the proposed sequential procedure, a NLP model was first formulated. This model consists of 81 constraints and 145 continuous variables. Solver CONOPT was adopted to carry out the corresponding optimization computation. The minimum freshwater supply rate was found to be 174.03 t/h within 0.1 CPU second. The first MINLP model was constructed with 162 constraints, 80 binary variables and 145 continuous variables and DICOPT was the selected solver. By setting TP to be zero, the minimum interconnection number was identified to be 19 within 2 CPU second. The resulting solution is shown in Figure 4 and Table 13. Finally, the minimum total throughput was determined to be 306.89 t/h with the second MINLP model. This model was solved with SBB in less than 0.6 CPU second. Notice that, due to convergence difficulties, solver DICOPT was not used in this example. The final solution is the same as the one obtained previously with the first MINLP Model. A comparison between the aforementioned and the published results is given in Table 14. It is clear that the network identified with the proposed method is better in terms of freshwater usage, number of matches and total throughput.

5.5. Example 5. This example deals with the design of water-using system in a petroleum refinery and the corresponding process data[18] are presented in Table 15. In this system, there are three contaminants, that is, (1) hydrocarbons (HC), (2) hydrogen sulfide (H_2S), and (3) salts, and seven fixed-load water users, that is, (1) atmospheric distillation unit (CDU), (2) hydrotreating unit (HDS), (3) crude desalter (Desalter), (4) cooling tower (CT), (5) boiler (Boiler), (6) delayed coker (Coker), and (8) the other operations (Others). A fixed water loss of 770 t/h is assumed for the evaporative cooling operation and there is no contaminant in the lost stream. In the reported optimal solution, there are 20 interconnections and the freshwater consumption rate is 1053.4 t/h .[18] This example was later studied by Liu et al.[24] Their final network featured 17 interconnections, but the corresponding freshwater consumption rate was raised to 1057.24 t/h.

The proposed NLP model was formulated with 71 constraints and 120 continuous variables, while the first MINLP model was constructed with 135 constraints, 63 binary variables and 120 continuous variables. CONOPT was adopted for solving the former model and BARON for the latter. The minimum freshwater consumption rate was found to be 1051.13 t/h within 0.1 CPU second. When TP = 0, the minimum interconnection number could be computed with the first MINLP model and this optimal value is 23. However, it was observed that the flow rates of 6 spent-water streams in the corresponding solution are less than 1 t/h and, therefore, this undesirable solution is not presented here for brevity.

For the purpose of eliminating the aforementioned negligible spent-water streams so as to compare the resulting design with the reported solutions, TP was reset to 2.27 and then to 6.11 t/h in the first MINLP. Consequently, the allowed freshwater supply rates were raised to 1053.4 and 1057.24 t/h respectively. The second MINLP model was also solved accordingly for each case. The main features of all aforementioned solutions are summarized in Table 16. From these results, it can be observed that the proposed sequential approach always yields much simpler networks at different levels of freshwater usage. For the sake of

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brevity, only the solution for TP = 6.11 t/h is presented in Figure 5 and Table 17.

6. CONCLUSIONS

A multiobjective optimization strategy has been developed in this work to generate appropriate designs for any water-using system with more than one contaminant. In particular, one NLP model and two MINLP models are solved in consecutive steps so as to satisfy three important criteria, that is, minimum freshwater usage, minimum interconnection number and minimum total throughput, as much as possible. Five examples are adopted in this paper to illustrate the implementation procedure. From the solutions obtained in these examples, it can be observed that more desirable network designs can usually be generated by the proposed approach.

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