Improved Optimization Strategies for Generating Practical Water-Usage and -Treatment Network Structures

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A design procedure to generate practical structures for the water-usage and -treatment networks is presented in this paper. The optimization strategies used in the proposed procedure are developed on the basis of a modified version of the existing nonlinear programming model. In particular, a systematic method is used to incorporate additional design options and a fixed number of repeated treatment units into the superstructure. Also, to account for the possible existence of unrecoverable solutes, the inequality constraints on their concentrations are added in the revised model formulation. To enhance convergence efficiency, a reliable method is developed in this work to produce a good initial guess. The advantages of this initialization technique are demonstrated with several examples adopted from the literature. Finally, several useful solution techniques to manipulate the structural properties of water networks are provided at the end of this paper. The effectiveness of our approach for creating favorable network structures is shown in the results of case studies.

Introduction

Despite of the fact that freshwater is an essential resource for running any chemical plant, it is actually in short supply in many regions of the world. Takama et al.[1] first studied the optimal water allocation problem in a refinery. A superstructure including all possible reuse options and network connections was built, and then an iterative decomposition procedure was used to solve the model. Later, the so-called pinch method was adopted by Wang and Smith[2,3] to design the water-using and wastewater-treatment networks separately. These pioneering works stimulated a series of enthusiastic research activities in recent years.[4−13] Notice that to avoid handling the complex interactions between water-using and wastewater-treatment networks, the earlier studies only focused on the design issues concerning either one of these two subsystems. An integrated approach for the overall system design remained a challenge until a general nonlinear programming (NLP) model was developed by Huang et al.[7] In a subsequent work, Tsai and Chang[10] adopted a genetic algorithm to identify the optimum solution of the same problem.

Although the above NLP model has been proven to be useful in creating optimal water-system designs on the basis of given objective functions, the resulting network structures may still be less than desirable in practical applications. This is due to the fact that it was not formulated to produce the *structural features* needed for effective operation of the overall water systems. It is therefore necessary to improve the present optimization strategies to meet this demand for obtaining the optimum solution while controlling the network configuration. Specifically, the following modifications have been introduced in the proposed design procedure:

(i) Because in certain applications the practices of self-looping around a water-using or wastewater-treatment unit and/or diluting the effluents at the discharge points may be acceptable and advantageous, the needed connections have been added to the superstructure to facilitate such design options.

(ii) Because the superstructure in the previous approach did not address the issue of repeated treatment units systematically, a short-cut method has been developed to determine the proper number of each unit to be embedded in the superstructure.

(iii) Because the structure of regeneration−recycle may cause accumulation of solutes that are not treatable in the recycle loop, additional model constraints have been imposed on their concentrations at the inlets and outlets of some of the water-using and water-treatment units.

(iv) Because, from a practical standpoint, it is often desirable to operate a "simple" water-usage and -treatment network (WUTN), a performance index reflecting structural simpleness has been devised and included in the objective function.

Notice also that the initial guess usually exerts a profound impact on the convergence of the search process in solving a NLP problem. A reliable method has thus been developed in this work to produce a good one. Specifically, a simple procedure has been proposed to connect the water-using and wastewater-treatment units in the superstructure to form an *initial structure* first. The water flow rate of each branch in this structure can then be easily chosen by inspection to satisfy the water balances on all mixing and splitting nodes. The remaining solute-balance equations can be uniquely solved for the pollutant concentrations as long

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as all flow rates are fixed. The advantages of this initialization technique are clearly shown with several examples adopted from the literature. Finally, the effectiveness of our optimization strategies for creating favorable network structures is demonstrated in the case studies presented at the end of this paper. In general, it can be said that the proposed improvements make the updated water network design method more general, robust, and easy to use.

Unit Models

To incorporate the above improvements in the design of WUTNs, it is necessary to revise the existing mathematical programming model accordingly. To facilitate understanding of the modified model formulations, let us introduce the definitions of two unit sets and a species set, i.e.

$$\mathbf{U} = \{u|u \text{ is the label of a water-using unit in the plant; } u = 1, 2, ..., N_U\} \quad (1)$$

$$\mathbf{T} = \{t|t \text{ is the label of a water-treatment unit in the plant; } t = 1, 2, ..., N_T\} \quad (2)$$

$$\mathbf{C} = \{k|k \text{ is the label of a solute that affects the water quality; } k = 1, 2, ..., N_C\} \quad (3)$$

To account for the fact that not all of the solutes in wastewater can be recovered, the species set is further divided into two subsets, i.e.

$$\mathbf{C} = \mathbf{C1} \cup \mathbf{C2} \quad (4)$$

where

$$\mathbf{C1} = \{k_1|k_1 \text{ is the label of a solute that can be recovered by at least one treatment unit; } k_1 = 1, 2, ..., N_{C1}\} \quad (5)$$

$$\mathbf{C2} = \{k_2|k_2 \text{ is the label of a solute that cannot be recovered by any treatment unit; } k_2 = 1, 2, ..., N_{C2}\} \quad (6)$$

Notice that

$$\mathbf{C1} \cap \mathbf{C2} = \varnothing \quad (7)$$

$$N_C = N_{C1} + N_{C2} \quad (8)$$

Although the modified models of water-using units and wastewater-treatment units in this work are actually very similar to those given by Tsai and Chang,[10] they are, nonetheless, outlined in the appendix for the sake of completeness. The revisions adopted in these models are mainly concerned with solutes in the set **C2**.

Water Sources and Sinks

Because our design objective is to optimize water distribution within a process plant, the scope of this study should be defined by the plant boundary. The external water sources can thus be categorized into two types, i.e., *primary waters* acquired from the environment and *secondary waters* obtained within the plant due to reaction and/or separation. On the other hand, all potential water sinks can be classified into three types on the basis of the present scope of optimization studies, i.e., the surface waters and groundwaters in the environment (type A), the common facilities for treating the effluents from various plants on the industrial park (type B), and the fictitious exit for collecting operation losses from both water-using and water-treatment units (type C).

On the basis of the above classification, the following five sets of labels can be defined:

$$\mathbf{I}_1 = \{p|p \text{ is the label of a primary source for WUTN; } p = 1, 2, ..., N_P\} \quad (9)$$

$$\mathbf{I}_2 = \{s|s \text{ is the label of a secondary source for WUTN; } s = 1, 2, ..., N_S\} \quad (10)$$

$$\mathbf{O}_A = \{a|a \text{ is the label of a type A sink for WUTN; } a = 1, 2, ..., N_A\} \quad (11)$$

$$\mathbf{O}_B = \{b|b \text{ is the label of a type B sink for WUTN; } b = 1, 2, ..., N_B\} \quad (12)$$

$$\mathbf{O}_C = \{c|c \text{ is the label of a type C sink for WUTN}\} \quad (13)$$

Superstructure

Similar to any other optimization study in process synthesis, it is necessary to build a superstructure in which all possible flow configurations are embedded. The superstructure adopted here is essentially the same as that suggested by Tsai and Chang[10] except for the following two new features:

(i) The primary waters are allowed to enter all water sinks directly to dilute the effluents. This option may be useful in certain applications when it is technically impossible to lower the concentration of a pollutant to its target level or its treatment cost is too prohibitive.

(ii) The self-looping recycle scheme around a water-using unit or a wastewater-treatment unit is adopted as an acceptable design option. This practice can be viewed as a way to reduce the use of makeup water while keeping the throughput above a given lower limit.

A simple construction procedure of the superstructure is presented below:

1. Place a mixing node at the inlet of every water-using unit and every water-treatment unit.
2. Place a mixing node before each type A and each type B sink.
3. Place a mixing node before a type C sink to collect loss streams from all water-using and water-treatment units.
4. Place a splitting node after each water source. The split branches from every such node are connected to all of the mixing nodes established in steps 1 and 2.
5. Place a splitting node at the exit of every water-using unit and every water-treatment unit. The split branches from every such node are connected to all of the mixing nodes installed in steps 1 and 2.

This scheme can be represented by Figure 1, in which the symbols S_p^P ($p \in \mathbf{I}_1$) and S_s^S ($s \in \mathbf{I}_2$) denote the splitting nodes after the pth primary source and the sth secondary source, respectively, M_a^A ($a \in \mathbf{O}_A$) and M_b^B ($b \in \mathbf{O}_B$) denote respectively the mixing nodes before sinks of type A and B, M^C denotes the mixing nodes before a

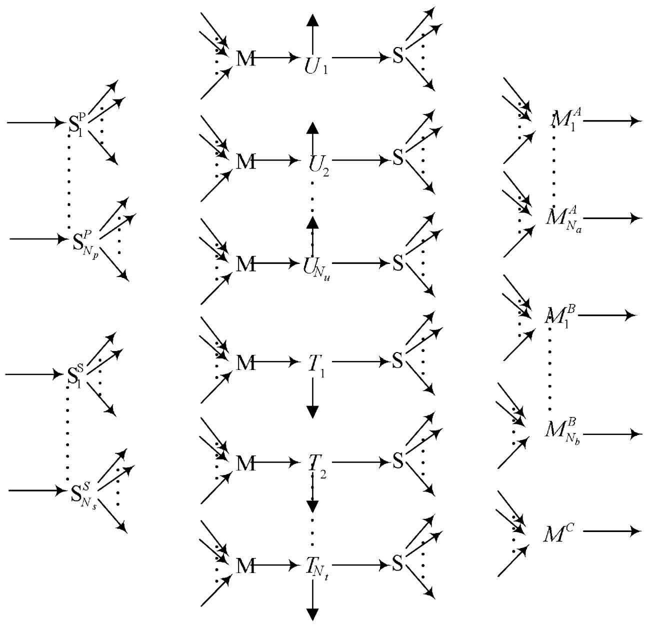

Figure 1. Generalized superstructure for the WUTNs.

type C sink, and $M - U_u - S$ ($u \in \mathbf{U}$) and $M - T_t - S$ ($t \in \mathbf{T}$) represent respectively the uth water-using unit and tth water-treatment unit with their attached mixing and splitting nodes. Notice that there is always one output from U_u or T_t that is not connected to the splitter on the exit. All such streams are connected to M^C.

Nodal Constraints

Other than the unit models described in the appendix, the water and solute balances around the splitting and mixing nodes in the superstructure must be imposed in the nonlinear program as equality constraints. To facilitate the subsequent presentation, the unit sets defined in eqs 1 and 2 can be combined; i.e.

$$\mathbf{P} = \mathbf{U} \cup \mathbf{T} \tag{14}$$

Because, in the superstructure, a splitting node is placed at the exit of every unit in $\mathbf{P}$ and every water source in $\mathbf{I}_1$ and $\mathbf{I}_2$, these nodes can be identified according to the labels of such units and sources. In other words, the set of all splitting nodes can be defined as

$$\mathbf{S} = \mathbf{P} \cup \mathbf{I}_1 \cup \mathbf{I}_2 \tag{15}$$

Similarly, because a mixing node is placed before every unit in $\mathbf{P}$ and every sink in $\mathbf{O}_A$, $\mathbf{O}_B$, and $\mathbf{O}_C$, the set of all mixing nodes can be defined as

$$\mathbf{M} = \mathbf{P} \cup \mathbf{O}_A \cup \mathbf{O}_B \cup \mathbf{O}_C \tag{16}$$

The water and solute balance equations can be formulated in a straightforward fashion around all of the splitting and mixing nodes included in $\mathbf{S}$ and $\mathbf{M}$. Because a complete version can be found elsewhere,[10] these equations are not presented explicitly here for the sake of brevity.

Objective Functions

The annualized cost of a WUTN is used as the objective function of the proposed NLP model. The general form of this cost function Φ can be written as

$$\Phi = \vartheta_w \Phi_w + \vartheta_o \Phi_o + \vartheta_c \Phi_c \tag{17}$$

where Φ_w, Φ_o, and Φ_c respectively denote the cost of primary waters, the operating cost, and the capital cost of a WUTN.

The freshwater cost can be expressed in a straightforward fashion as

$$\Phi_w = \sum_{p \in \mathbf{I}_1} \omega_p^w \bar{F}_p \tag{18}$$

where $\bar{F}_p$ and ω_p^w denote respectively the consumption rate and the cost per unit mass of the pth primary water.

For computation convenience, the operating cost of a WUTN is approximated according to the following equation:

$$\Phi_o = \sum_{u \in \mathbf{U}} \omega_u^U F_u + \sum_{t \in \mathbf{T}} \omega_t^T F_t + \sum_{b \in \mathbf{O}_B} \omega_b^d F_b \tag{19}$$

where F_u and F_t denote respectively the throughputs in the uth water-using unit and the tth water-treatment unit, F_b represents the discharge rate to the bth type B sink, and ω_u^U, ω_t^T, and ω_b^d are constant cost coefficients.

In this work, it is assumed that the total capital cost of a WUTN consists mainly of treatment-unit costs and piping costs,[1,14] i.e.

$$\Phi_c = \sum_{t \in \mathbf{T}} \omega_t^c F_t^{0.7} + \sum_{i \in \mathbf{S}, j \in \mathbf{M}} \omega_{ij}^p f_{ij}^{0.6} \tag{20}$$

where ω_t^c is the capital-cost coefficient of the tth water-treatment unit, f_{ij} is the water flow rate from splitting node i to mixing node j, and ω_{ij}^p is the corresponding cost coefficient. Notice that the plant layout is assumed to be fixed in this case. Because the locations of all water-using and water-treatment units are selected in advance, the piping cost is affected only by the flow rates f_{ij} and the length of each pipe is reflected in the constant cost coefficient ω_{ij}^p.

Naturally, it may not be necessary to consider all types of costs in every application. A binary value of 0 or 1 can be assigned to each weighting factor in eq 17 on a case-by-case basis. For example, one may want to neglect the capital cost (i.e., $\vartheta_c = 0$) in a revamp study. It should also be noted that the network structure can be effectively manipulated by judicially selecting these weighting factors. It is obvious that the regeneration–recycle and regeneration–reuse structures are the dominant network characteristics if water conservation is emphasized in WUTN design; i.e., $\vartheta_w = 1$ and $\vartheta_o = \vartheta_c = 0$. On the other hand, if network simplicity is the design goal, then it may be advantageous to set $\vartheta_c = 1$ and $\vartheta_w = \vartheta_o = 0$ and increase the values of piping-cost coefficients ω_{ij}^p.

Repeated Treatment Units in a Superstructure

Generally speaking, the operating conditions of all water-using units are determined by the process requirements. In other words, these units exist as a part of the chemical process itself. On the other hand, the water-treatment units in a superstructure can be viewed as the offline equipments available for possible installation. As long as the environmental regulations are satisfied, the number of each repeated units used in the actual network may be less than that in the superstructure and it may not even be necessary to use every type of available treatment unit in the *optimum* solution.

Obviously, the numbers of repeated treatment units in the superstructure must be specified before constructing the NLP model. These numbers should be large enough to ensure adequate search space but not too large to impede computation. In this study, the number of each type of repeated treatment unit is set with heuristic rules so that these repeated units alone can be used (1) to accommodate all wastewater streams and (2) to lower the pollutant concentrations to their target values at discharge points or inlets of water-using units. These heuristics were developed on the basis of an assumption that every wastewater stream in the water network, from either a water-using unit or a secondary water source, can be treated by at least one type of available treatment unit. This assumption limits the possibilities that have to be considered in estimating the total flow rate of wastewater and thus greatly simplifies the implementation steps. A detailed description of these rules is presented below:

(i) Rule 1. For a treatment unit characterized by the constant outlet concentration of a single solute, the number of repeated units is set as 1 if there is no upper throughput limit. Otherwise, the number of repeated units, n_j^{unit}, should be the same as the number of parallel units to process all wastewaters. The latter is the smallest positive integer that satisfies the following constraint:

$$n_j^{\text{parallel}} \geq \frac{1}{\eta_j}\left(\sum_{s\in\mathbf{I}_2}\bar{F}_s + \sum_{u\in\mathbf{U}}\bar{F}_u\right) \qquad j \in \mathbf{T} \tag{21}$$

where n_j^{parallel} is the number of parallel units, $\bar{F}_s$ is the generation rate of the sth secondary water, $\bar{F}_u$ is the output flow rate of the uth water-using unit, and η_j is the upper throughput limit of the jth water-treatment unit.

(ii) Rule 2. For a treatment unit characterized by the removal ratio ψ_j of a single solute, a simple hand calculation procedure can be devised on the basis of eq A12 to determine the number of stages, n_j^{stage}, needed to reduce the solute concentration from its highest possible value in a WUTN, $C_{\text{source}}^{\max}$, to the lower bound, $C_{\text{sink}}^{\min}$. Specifically, n_j^{stage} should be the smallest positive integer that satisfies the following constraint:

$$(1-\psi_j)^{n_j^{\text{stage}}} \leq \frac{C_{\text{sink}}^{\min}}{C_{\text{source}}^{\max}} \qquad j \in \mathbf{T} \tag{22}$$

It should be noted that the water-treatment system in a WUTN is in essence a waste interception network (WIN) in the process plant.[15] The sources of the WIN are wastewaters generated from water-using units and also the secondary waters of a WUTN. On the other hand, the sinks of the WIN can be considered to be the type A and B sinks of a WUTN and also the water-using units. Thus, $C_{\text{source}}^{\max}$ should be chosen as the maximum value among the solute concentrations of secondary waters and also the upper bounds of the outlet concentrations of all water-using units; $C_{\text{sink}}^{\min}$ should be the minimum value among the upper bounds of the solute concentrations at water sinks and also the inlets of water-using units.

The number of parallel trains of treatment units, n_j^{parallel}, can be determined with the approach described in rule 1. The total number of repeated units n_j^{unit} can then be calculated accordingly, i.e.

$$n_j^{\text{unit}} = n_j^{\text{stage}}\, n_j^{\text{parallel}} \qquad j \in \mathbf{T} \tag{23}$$

(iii) Rule 3. For a multiple-solute treatment unit, different unit numbers may be obtained by following either rule 1 or rule 2 on the basis of the process data of different solutes. To avoid incorporating an unnecessarily large number of repeated units in the superstructure, a heuristic is adopted in this work to select one of these computed numbers; i.e., the chosen value of n_j^{unit} should be the largest one among those that are not more than 3 times the smallest number.

Two examples are presented in the sequel to illustrate the implementation steps of the above rules.

Example 1. This example is taken from Kuo and Smith,[5] in which three solutes, i.e., hydrocarbon (H.C.), H_2S, and suspended solids (S.S.), are considered in the WUTN design for a refinery. There is only one water source and one type A sink in this network. The primary water is assumed to be pure, and the upper limits of discharge pollutant concentrations are 20, 5, and 100 ppm for the above three solutes, respectively. The process data of five existing water-using units are listed in Table 1. Notice that these units can be described with eqs A1 and A3 under the condition that $\nu_i = 0$. The process data of three available water-treatment units are given in Table 2. Notice that these treatment units are modeled according to eqs A8−A14 and none of these operations result in water loss, i.e., $\phi_j = 0$.

On the basis of the process data given in Table 1, the highest possible source concentration of H.C. is 220 ppm, which is the concentration at the exit of the desalter (U3). Similarly, it can be observed that the

Table 1. Process Data of the Water-Using Units in Example 1

unit no.	solute	mass load μ_{ik} (kg/h)	max inlet concn β_{ik} (ppm)	max outlet concn γ_{ik} (ppm)
steam stripping (U1)	H.C.	0.75	0	15
	H_2S	20.00	0	400
	S.S.	1.75	0	35
hydrodesulfurization I (U2)	H.C.	3.40	20	120
	H_2S	414.80	300	12500
	S.S.	4.59	45	180
desalter (U3)	H.C.	5.60	120	220
	H_2S	1.40	20	45
	S.S.	520.80	200	9500
ejector stream for vacuum column (U4)	H.C.	0.16	0	20
	H_2S	0.48	0	60
	S.S.	0.16	0	20
hydrodesulfurization II (U5)	H.C.	0.80	50	150
	H_2S	60.80	400	8000
	S.S.	0.48	60	120

Table 2. Process Data of the Water-Treatment Units in Example 1

	removal ratio (%)		
unit no.	H.C.	H_2S	S.S.
T1	0	99.9	0
T2	70	90	98
T3	95	0	50

Table 3. Water Sources of the Process in Example2

source no.	concn (ppm) solute A	solute B	max flow rate (tons/h)
W1	0.1	0.1	∞
W2	60.0	28.0	30.0
W3	1800.0	1200.0	40.0

Table 4. Process Data of the Water-Using Units in Example 2

unit no. (Ui)	solute (k)	mass load μ_{ik} (kg/h)	max inlet concn β_{ik} (ppm)	max outlet concn γ_{ik} (ppm)	water loss ν_i (tons/h)
U1	A	8.0	0.1	100.1	0
	B	4.0	25.0	75.0	
U2	A	11.2	80.0	240.0	0
	B	4.2	30.0	90.0	
U3	A	0.0	8.0	8.0	15.0
	B	0.0	5.0	5.0	

maximum source concentrations of H_2S (at the exit of U2) and S.S. (at the exit of U3) are 12500 and 9500 ppm, respectively. The lowest possible sink concentrations can be identified by comparing the upper concentration limits at the discharge point and also the inlets of water-using units. For H.C., H_2S, and S.S., these values are 20, 5, and 45 ppm, respectively.

Let us consider the treatment unit T1 first. Notice that T1 can only be used to remove solute H_2S. According to rule 2, the corresponding number of stages must satisfy the following constraint:

$$12500(1 - 0.999)^{n_1^{\text{stage}}} \leq 5$$

Thus, n_1^{stage} for H_2S should be 2. Also, because there is no throughput limit, $n_1^{\text{parallel}} = 1$ and therefore $n_1^{\text{unit}} = n_1^{\text{stage}} = 2$. On the other hand, because the removal ratios for H.C. and S.S. in T1 equal zero, the corresponding numbers of stages and units can both be considered as approaching infinity. Thus, on the basis of the third heuristic rule, we should adopt two T1s in the superstructure.

The numbers of T2s in the superstructure can be computed with essentially the same procedure. The numbers of stages to remove H.C., H_2S, and S.S. can be found as 2, 4, and 2, respectively. Consequently, $n_2^{\text{unit}} = 4$. Finally, notice that H_2S cannot be removed by T3, and thus the corresponding number of repeated units can be considered to be a very large positive value. On the other hand, the numbers of stages needed to remove H.C. and S.S. with T3 can be determined as 1 and 8, respectively. In this case, because the required stage numbers for H_2S and S.S. are much larger than that for H.C., only one T3 should be adopted in the superstructure.

Example 2. This example is adopted from Tsai and Chang.[10] The properties of three water sources considered here are listed in Table 3. Notice that only the first is a primary water and its supply is unlimited. There is only one sink, and the maximum allowable concentrations of the two key solutes are both 10 ppm. The process data of three existing water-using units in a WUTN are presented in Table 4, and eqs A1−A7 can be used to formulate the corresponding unit models. In the cases of U1 and U2, the mass loads are specified and $\nu_1 = \nu_2 = 0$. On the other hand, because there is a water loss of 15 tons/h in the third unit U3, two additional equality constraints, which are expressed in

Table 5. Process Data of the Water-Treatment Units in Example 2

unit no. (Tj)	solute (k)	removal ratio ψ_{jk}	max inlet concn β_{jk} (ppm)	constant outlet concn λ_{jk} (ppm)	max throughput η_j (tons/h)
T1	A	0.9			125.0
	B	0.1			
T2	A	0.2			125.0
	B	0.95			
T3	A		200.0	5.0	125.0
	B		100.0	5.0	

the form of eq A4, should be imposed upon the solute concentrations in the loss stream. The process data of three types of available water-treatment units are given in Table 5. These units can be described with eqs A8−A17. The water losses in all three units are considered to be negligible, i.e., $\phi_1 = \phi_2 = \phi_3 = 0$. Notice that the removal ratios of T1 and T2 are specified in Table 5. Thus, the four additional equations associated with eq A12 should be included in the mathematical program. Notice also that the exit concentrations of T3 are assumed to be constant in this example. The two corresponding constraints should be formulated according to eq A15.

In contrast to example 1, there are two secondary water streams, W2 and W3, in this problem, and thus the solute concentrations in these streams should also be treated as the source concentrations of WIN. On the basis of the data given in Tables 3 and 4, the maximum source concentrations of solutes A and B should be 1800 and 1200 ppm, respectively, and the minimum sink concentrations should be 0.1 and 5 ppm, respectively.

Because there are throughput limits on the treatment units, the highest possible wastewater flow rate should be estimated. It is clear that this flow can be produced if the requirements of all water-using units are satisfied with primary water *only*. Thus, the wastewater flow rate generated from each water-using unit can be estimated on the basis of eqs A1, A3, and A4, in which C_{ik}^{in} is set as the concentration of solute k in a primary water and C_{ik}^{out} the concentration of upper bound γ_{ik} at the outlet of this water-using unit. If there are several solutes involved, the largest estimate should be used in the subsequent calculations. Let us first try to use the above approach to estimate the wastewater produced in U1. Because there is no water loss, the unit model can be rearranged as

$$\bar{F}_1 = \frac{\mu_{1k}}{\gamma_{1k} - C_k^{\text{W1}}} \qquad k \in \mathbf{C1} \tag{24}$$

where C_k^{W1} is the concentration of solute k in primary water. Thus, the wastewater flow rate of unit U1 can be estimated as 80 tons/h on the basis of the mass load of solute A, while this estimate is 53 tons/h if the mass load of solute B is adopted as the basis of calculation. Similarly, the wastewater production rates of U2 and U3 can be estimated as 46.7 and 15.3 tons/h, respectively. Therefore, the maximum total flow rate of wastewater is 80 + 46.7 + 15.3 + 30 + 40 = 212 tons/h. Notice that this flow rate exceeds the throughput limit of every available treatment unit in this example. By applying rule 1 or rule 2, we can find that $n_1^{\text{parallel}} = n_2^{\text{parallel}} = n_3^{\text{parallel}} = 2$.

Next, let us try to determine the number of T1s in the superstructure. The number of stages can be com-

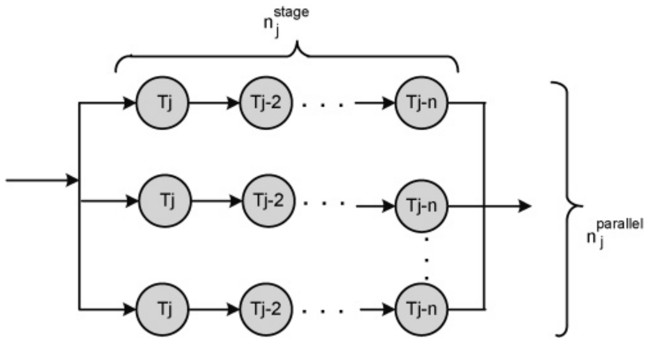

Figure 2. Substructure of the *j*th type of treatment units.

puted on the basis of the removal ratio of either solute A or solute B. It was found that $n_1^{\mathrm{stage}} = 5$ in the former case and $n_1^{\mathrm{stage}} = 52$ in the latter. By application of rule 3, the following selection can be made:

$$n_1^{\mathrm{unit}} = n_1^{\mathrm{stage}}\, n_1^{\mathrm{parallel}} = 5 \times 2 = 10$$

By following the same procedure, the numbers of T2s and T3s in the superstructure can be determined as 4 and 2, respectively.

Initial Guess

While the search space of the proposed NLP problem is defined by the superstructure, the starting point of the iterative solution procedure is provided by an initial guess. The initial guess usually exerts a profound influence on the convergence of the search process. After trying different initial guesses for each example in this study, we recommend a method to produce an initial guess for the NLP model, which requires little data to be provided and leads to an optimal solution in most cases. The initial guess is produced in three steps, i.e., (1) constructing an initial network structure, (2) selecting the feasible flow rate of every branch in the initial structure to satisfy water balances, and (3) solving a set of linear equations for the inlet and outlet concentrations of each unit in the initial structure. It should be noted that step 3 can be easily realized by calling any available linear programming solver.

The initial structure of a WUTN is built according to the following procedure:

1. Connect each water-using unit to an arbitrarily selected primary water source.

Table 6. Cost Functions of the Treatment Units Used in Example 3

T1	capital cost ($US)	$16800F^{0.7}$
	operating cost ($US/h)	F
T2	capital cost ($US)	$12600F^{0.7}$
	operating cost ($US/h)	$0.0067F$
T3	capital cost ($US)	$4800F^{0.7}$
	operating cost ($US/h)	0

2. Combine all secondary waters and the wastewaters from all water-using units into one stream.

3. Construct a substructure for the *j*th type of treatment units according to Figure 2, in which n_j^{parallel} trains of repeated units are connected in parallel and n_j^{stage} units are connected in series in each train. Repeat the present step for $j = 1, 2, ..., N_{\mathrm{T}}$.

4. Connect all substructures in series and then attach the resulting water-treatment network to the combined wastewater stream established in step 2.

A solution of the proposed NLP model, in general, contains the flow rate of each branch in a WUTN and also the inlet and outlet concentrations of each unit. If the flow rates are fixed, the concentrations can be uniquely determined by solving the solute balance equations. This assertion can be verified by an analysis of the degree of freedom in the NLP model. Notice that, although the *feasible* flow rates in the initial structure can be easily selected to satisfy the water balances, some of the corresponding concentrations may be infeasible. This is, nonetheless, acceptable in most NLP solvers as long as the violations of inequality constraints are not "serious".

The following examples are adopted to show that the proposed initialization procedure, in general, facilitates reliable and efficient convergence in the search process. All models in this study were built in GAMS[16] and solved with module *conopt2*.

Example 3. Let us consider the design problem described in example 1 again. The cost functions of treatment units in this example are presented in Table 6. It is assumed that (1) the freshwater cost is 0.2 $US/ton, (2) the annual depreciation rate is 10%, and (3) the plant operates 8600 h/year. For comparison purposes, the weighting factors used in the present case are the same as those reported in Kuo and Smith,[5] i.e., $\vartheta_{\mathrm{w}} = \vartheta_{\mathrm{o}} = \vartheta_{\mathrm{c}} = 1$ and $\omega_u^{\mathrm{U}} = \omega_{ij}^{\mathrm{p}} = 0$. After an initial guess is obtained according to the proposed method, the optimal WUTN can then be generated with the NLP model. The solution is shown in Figure 3 and Table 7. The discharge

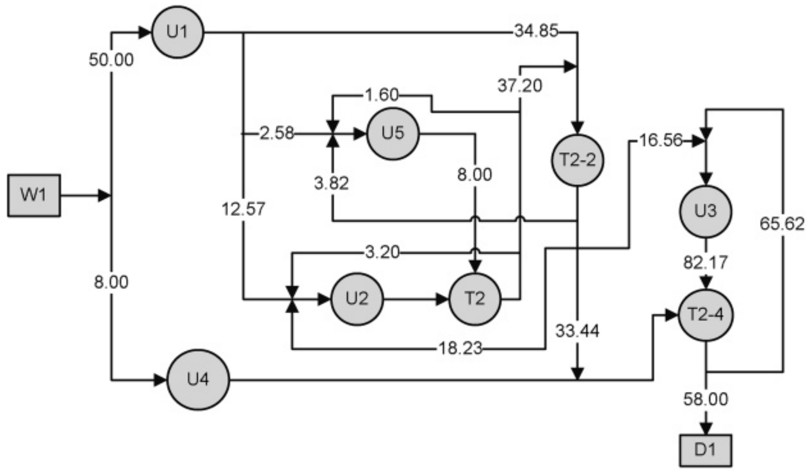

Figure 3. Optimal solution obtained in example 3.

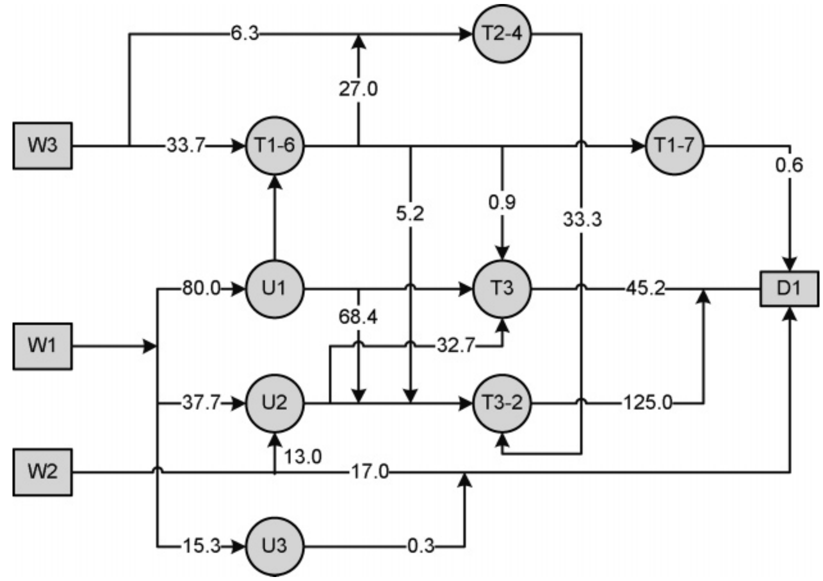

Figure 4. Optimal solution obtained in example 4.

Table 7. Optimal Operating Conditions of the Process Units in Example 3

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U1	50.0	H.C.	0	15.0
		H_2S	0	400.0
		S.S.	0	35.0
U2	34.0	H.C.	12.7	112.7
		H_2S	300.0	12500.0
		S.S.	13.4	148.4
U3	82.2	H.C.	15.6	83.8
		H_2S	20	37.0
		S.S.	68.1	6405.6
U4	8.0	H.C.	0	20.0
		H_2S	0	60.0
		S.S.	0	20.0
U5	8.0	H.C.	15.2	115.2
		H_2S	400.0	8000.0
		S.S.	12.0	72.0
T2	42.0	H.C.	113.2	34.0
		H_2S	11642.9	1164.3
		S.S.	133.8	2.7
T2-2	72.0	H.C.	24.8	7.4
		H_2S	794.6	79.5
		S.S.	18.3	0.4
T2-4	123.6	H.C.	59.0	17.7
		H_2S	50.0	5.0
		S.S.	4259.5	85.2

concentrations of H.C., H_2S, and S.S. in this design are 17.7, 5.0, and 85.2 ppm, respectively. Notice that the corresponding optimal cost is 192.63 × 10^3 \$US/year. When compared with the minimum cost obtained by Kuo and Smith,[5] i.e., 677.7 × 10^3 \$US/year, there is a 71.6% reduction.

Example 4. The process data given in example 2 are adopted here for the WUTN design. To compare our results with those given by Tsai and Chang,[10] the total operating cost defined in eq 19 (with $\omega_u^{\mathrm{U}} = \omega_t^{\mathrm{T}} = \omega_b^{\mathrm{d}} = 1$) is used as the objective function in the present example. Before formulation of the NLP model, it is imperative to remove the direct connections between the primary waters and the sinks in the superstructure. This is due to the fact that, if water source W1 is permitted to dilute the effluents, the use of treatment units becomes unnecessary because the freshwater cost is not present in the objective function.

Using the proposed initialization method, one can obtain the optimal solution shown in Figure 4 and Table

Table 8. Optimal Operating Conditions of the Process Units in Example 4

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U1	80.0	A	0.1	100.1
		B	0.1	50.1
U2	50.8	A	15.5	236.1
		B	7.3	90.0
U3	15.3	A	0.1	5.0
		B	0.1	5.0
T1-6	33.7	A	1800.0	180.0
		B	1200.0	1080.0
T1-7	0.6	A	180.0	18.0
		B	1080.0	972.0
T2-4	33.3	A	485.7	388.5
		B	1102.6	55.1
T3	45.2	A	200.0	5.0
		B	100.0	5.0
T3-2	125	A	200.0	5.0
		B	100.0	5.0

Table 9. Process Data of the Water-Using Units in Example 5

unit	flow rate (tons/h)	loss (tons/h)	inlet concn (ppm)	outlet concn (ppm)
reactor (U1)	80.0	60.0	100	1000
cyclone (U2)	50.0	0	200	700
filtration (U3)	10.0	−30.0	0	100
steam system (U4)	10.0	0	0	10
cooling system (U5)	15.0	10.0	10	100

8. The discharge concentrations of solutes A and B were both found to be 10.0 ppm. The corresponding value of the objective function is 383.87, which represents a 22.7% reduction from the reported value of 496.7.[10]

Example 5. Let us consider a water-using system design problem studied by Wang and Smith,[17] in which a fixed flow rate is required for each water-using unit. The process data of this system are presented in Table 9. Notice that only one solute, i.e., the suspended solid, affects the water quality. Note also that the loss rate of water in U3 is negative because there is a net gain in this operation. The design objective here is to minimize the freshwater usage. By solving the proposed NLP model, one can quickly obtain the optimal network shown in Figure 5. Notice that its freshwater consumption rate is the same as the reported value, i.e., 90.6 tons/h. Furthermore, several other optional designs with identical performances (e.g., see Figure 6) can also be

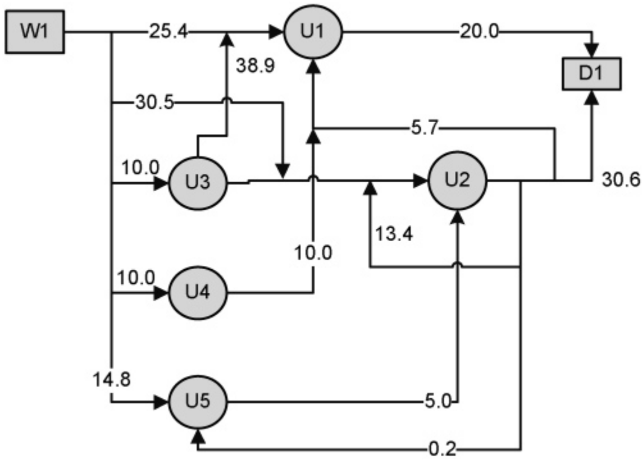

Figure 5. First optimal solution obtained in example 5.

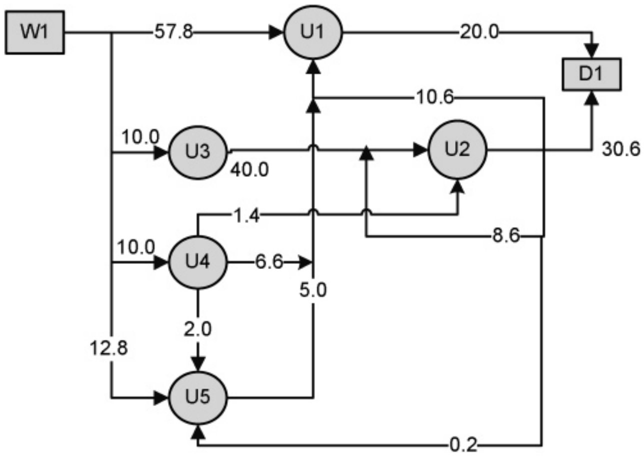

Figure 6. Second optimal solution obtained in example 5.

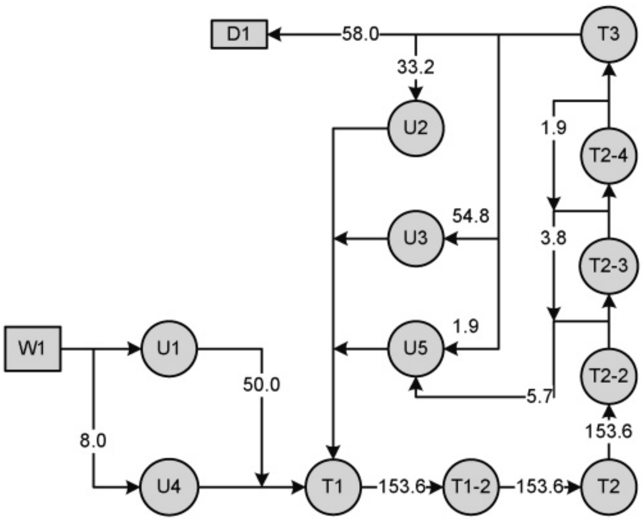

Figure 7. Solution of case 1: the optimal network requiring the least amount of freshwater.

easily generated by slightly varying the initial flow rates in the initial guess.

It is also worth noting that, when the throughput of a water-using or water-treatment unit is required to be maintained at a fixed flow rate or above a given lower limit, then the self-looping structures must be included in the superstructure to provide opportunities to reduce freshwater usage. Notice that a self-looping structure appears around U2 in Figure 5. If the practice of self-looping is not allowed in the present example, the water consumption rate will increase to 93.0 tons/h.

Impacts of Objective Functions

As mentioned before, the network structure can be effectively manipulated by judicially selecting the objective function of a nonlinear program. To illustrate the impacts of objective functions, the design problem in example 3 has been solved repeatedly in a series of case studies with the same superstructure and initial guess. The following is a brief summary:

1. $\Phi = \Phi_w$. The solution is shown in Figure 7. The freshwater requirement of this design is 58.0 tons/h and the discharge concentrations of H.C., H_2S, and S.S. are 0.03, 0, and 0 ppm, respectively. Notice that all seven treatment units in the superstructure are included in this WUTN. Also, the total number of branches in the optimal water network is 20 and that of recycle loops is 6.

2. $\Phi = \Phi_o$. The solution is shown in Figure 8. When $\omega_u^U = \omega_t^T = 1$ and $\omega_b^d = 0$, a minimum objective value of 296.93 can be obtained in this case and the corresponding discharge concentrations of the three pollutants are 20, 5, and 100 ppm, respectively. It can be observed from Figure 8 that, although T2-3 and T2-4 are embedded in the superstructure, they are excluded in the optimal WUTN design and the number of treatment units is 5. Notice also that the total number of branches in this water network is 23 and that of recycle loops is 2.

3. $\Phi = \Phi_c$. By neglecting the piping cost and setting the cost coefficients ω_t^c according to Table 6, one can obtain the optimal solution presented in Figure 9. The corresponding capital cost is 56.86×10^3 \$US/year, and the discharge concentrations are 20, 5, and 100 ppm, respectively. Notice that none of the treatment units are repeated in this design and the number of treatment units is only 3. Finally, notice that the total number of branches is 19 and that of recycle loops is 2.

From the results obtained in the above case studies, a number of interesting observations can be made.

(i) The number of recycle loops in the network obtained by minimizing the water consumption rate is the largest among the three. This is really not surprising because the recycles usually facilitate water conservation and no penalties on the operating or capital costs are included in the objective function.

(ii) The fewest treatment units are used in the network achieving minimum capital cost. This result can be attributed to the cost function given in the first term on the right-hand side of eq 20. Notice that, with an exponent of 0.7, this term favors the use of fewer units for processing the same throughput.

(iii) The number of branches in case 3 is also minimum. This is probably due to the fact that the fewest treatment units are used in this network.

Complexity Reduction Measures

The WUTN design obtained on the basis of eq 17 is cost-oriented. From a practical standpoint, it is also necessary to reduce the complexity of the water network in order to ensure operability and controllability. In this study, two simple measures are taken to modify the NLP model for this purpose:

(i) Place additional weight on the piping cost in the objective function.

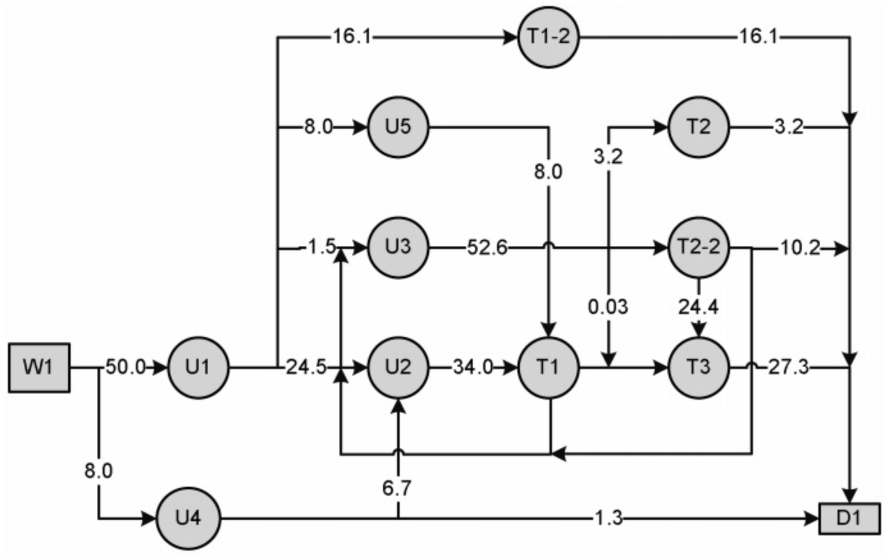

Figure 8. Solution of case 2: the optimal network requiring the minimum operating cost.

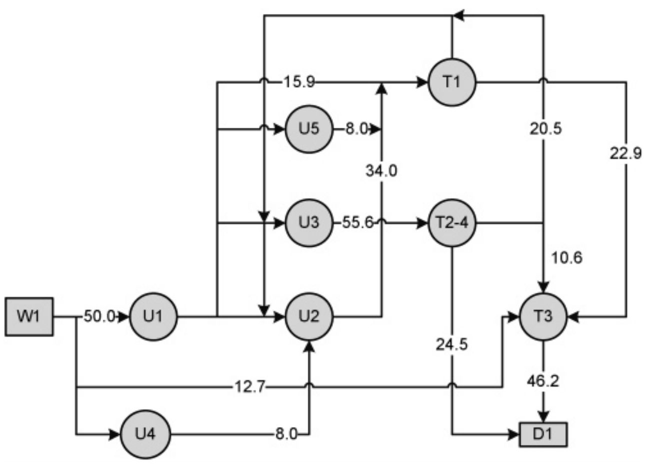

Figure 9. Solution of case 3: the optimal network requiring the minimum capital cost.

Obviously, the number of branches in the optimal water network can be reduced by increasing the values of ω_{ij}^{p} in eq 20. Let us use example 3 to illustrate the effects of this practice. If we change the values of ω_{ij}^{p} from 0 to 1 and solve the NLP model again, the total number of branches in the resulting WUTN (see Figure 10) can be reduced from 18 in the original design (see Figure 3) to 15.

(ii) Impose stringent constraints upon the concentration of an unrecoverable solute.

If an unrecoverable species is present in a regeneration–recycle structure, a purge stream must be provided to avoid accumulation of this material in the loop. This feature can be easily produced with the proposed model. Let us first consider a modified version of the design problem described in example 3. In this case, there exists an additional salt in the water source, and its concentration is 10 ppm. It is assumed that, although there is no discharge limit, the presence of this solute affects the performance of every water-using unit. Consequently, the upper bounds of salt concentrations at the inlet and outlet of each unit must be stipulated according to Table 10. The optimal solution can be found in Figure 11 and Table 11. The corresponding cost is 270.66×10^3 \$US/year, and the discharge concentrations of H.C., H_2S, S.S., and salt are 16.0, 5.0, 87.8, and 65.1 ppm, respectively. A comparison between Figure 3 (obtained in Example 3) and the present solution reveals that the primary water usage is raised from 58.0

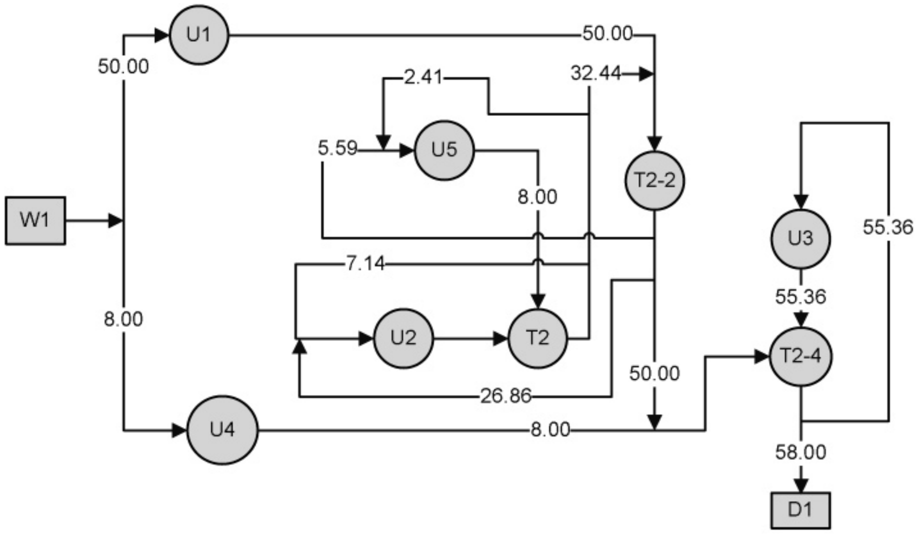

Figure 10. Optimum solution of example 3 obtained by placing additional weight on the piping cost.

Table 10. Additional Constraints on the Salt Concentrations in Example 3

unit no.	mass load μ_{ik} (kg/h)	max inlet concn β_{ik} (ppm)	max outlet concn γ_{ik} (ppm)
steam stripping (U1)	1.50	20	50
hydrodesulfurization I (U2)	2.38	30	100
desalter (U3)	1.12	30	50
ejector stream (U4)	0.08	20	30
hydrodesulfurization II (U5)	0.40	50	100

Table 11. Optimal Operating Conditions of the Process Units in Example 3 (Obtained with Process Data in Tables 1 and 10)

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U1	50.0	H.C.	0	15.0
		H_2S	0	400.0
		S.S.	0	35.0
		salt	10	40.0
U2	34.0	H.C.	13.5	113.5
		H_2S	249.4	12449.4
		S.S.	25.3	160.3
		salt	30.0	100
U3	55.0	H.C.	5.7	107.5
		H_2S	1.8	27.2
		S.S.	31.3	9500.0
		salt	29.6	50.0
U4	8.0	H.C.	0	20.0
		H_2S	0	60.0
		S.S.	0	20.0
		salt	10	20.0
U5	36.3	H.C.	14.9	36.9
		H_2S	400.0	2074.7
		S.S.	26.3	39.5
		salt	50.0	61.0
T2	70.3	H.C.	74.0	22.2
		H_2S	7092.0	709.2
		S.S.	97.9	2.0
		salt	79.9	79.9
T2-2	68.5	H.C.	21.9	6.6
		H_2S	695.7	69.6
		S.S.	3.4	0.1
		salt	78.1	78.1
T2-3	119.0	H.C.	53.2	16.0
		H_2S	50.0	5.0
		S.S.	4390.9	87.8
		salt	65.1	65.1

tons/h in the former design to 99.4 tons/h in the latter and the number of loops is reduced from 5 to 3. Such differences can certainly be attributed to the additional concentration constraints imposed in the NLP model.

If the effects of the salt on the performance of each water-using unit are unknown or uncertain, then it may

Table 12. Stricter Constraints on the Salt Concentrations Added in Example 3

unit no.	mass load μ_{ik} (kg/h)	max inlet concn β_{ik} (ppm)	max outlet concn γ_{ik} (ppm)
steam stripping (U1)	1.50	20	50
hydrodesulfurization I (U2)	2.38	10	80
desalter (U3)	1.12	10	30
ejector stream (U4)	0.08	20	30
hydrodesulfurization II (U5)	0.40	10	60

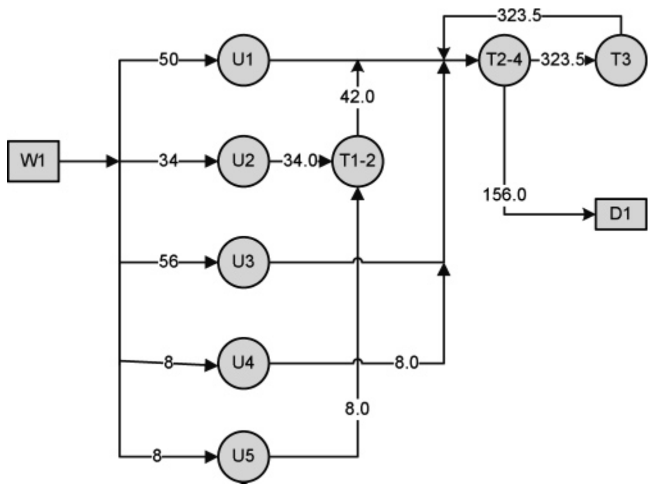

Figure 12. Another optimum solution of example 3 obtained by imposing stricter constraints on the concentration of the unrecoverable salt.

be necessary to impose stricter constraints to remove the regeneration−recycle or self-looping structures as much as possible. Let us change the upper bounds of the salt concentrations in Table 10 to those given in Table 12. The optimal solution in this case is shown in Figure 12. It can be observed that all of the regeneration−recycle and self-looping structures around water-using units are eliminated.

Conclusions

Improved optimization strategies are presented in this paper to generate practical structures for the WUTNs. A number of modifications are introduced into the NLP model formulations. In particular, they are the following:

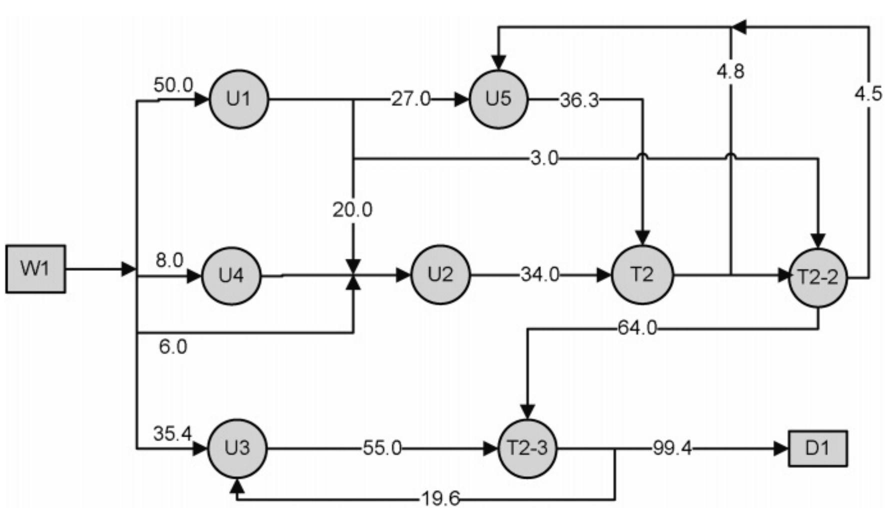

Figure 11. Optimum solution of example 3 by imposing additional constraints on the concentration of the unrecoverable salt.

(i) Additional design options, e.g., dilution at the discharge point and self-looping around a process unit, are incorporated in the superstructure.

(ii) A set of heuristical rules are proposed to determine the number of each type of repeated treatment units to be embedded in this superstructure.

(iii) To account for the possible existence of unrecoverable solutes, the inequality constraints on their concentrations are added in the revised model.

A reliable method is developed in this work to produce a good initial guess. The advantages of this initialization technique are clearly demonstrated with several examples adopted from the literature. Several useful solution techniques to manipulate the structural properties of WUTNs are also provided at the end of this paper. The effectiveness of our approach for creating favorable network structures is shown in the results of case studies. In general, it can be said that the proposed improvements make the updated water network design method more general, robust, and easy to use.

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Appendix: The Unit Models

The equipments considered in the present study are divided into two categories, i.e., water-using units and water-treatment units. Although more elaborate design equations for these units are available, only mass balances are considered here for the sake of simplicity in formulation. A brief description of the proposed unit models is presented in the sequel:

Water-Using Units. Basically, material balances for water and the solutes should be satisfied around each water-using unit. Specifically, water balance equations can be written as

$$F_i = \bar{F}_i + \nu_i \qquad i \in \mathbf{U} \tag{A1}$$

where F_i and F_i denote respectively the water flow rates at the inlet and outlet of unit i and ν_i is the operation loss. An alternative formulation of eq A1 can be written as

$$(1 - \theta_i)F_i = \bar{F}_i \qquad i \in \mathbf{U} \tag{A2}$$

where θ_i represents the fraction of water loss in unit i. Notice that, to provide an accurate description of the mathematical program, Greek symbols of lower case will be specially reserved for the design parameters throughout this paper.

In addition to water balances, it is necessary to consider the solutes that affect water quality, i.e.

$$F_iC_{ik}^{\mathrm{in}} + \mu_{ik} = \bar{F}_iC_{ik}^{\mathrm{out}} + \nu_iD_{ik} \qquad i \in \mathbf{U} \qquad k \in \mathbf{C} \tag{A3}$$

where C_{ik}^{in} and C_{ik}^{out} represent respectively the concentrations of solute k at the inlet and outlet of the water-using unit i, D_{ik} is the concentration of solute k in the loss stream, and μ_{ik} is the mass load of solute k in unit i.

In general, eqs A1 and A3 are sufficient for describing the units without water loss. However, additional constraints must be included to model the other operations properly. The simplest technique used in this work is to assume that the concentration of solute k in the lost stream is zero, i.e.

$$D_{ik} = 0 \qquad i \in \mathbf{U} \qquad k \in \mathbf{C} \tag{A4}$$

For example, the amount of nonvolatile inorganics in the leaked steam is indeed negligible. In other situations, it may be more appropriate to assume that the outlet concentration of a solute k is constant because it is dependent only on the operating conditions of the unit, i.e.

$$C_{ik}^{\mathrm{out}} = \lambda_{ik} \qquad i \in \mathbf{U} \qquad k \in \mathbf{C} \tag{A5}$$

where λ_{ik} is a constant and also a design parameter. An example of this case is the volatile organics at the exit of a cooling tower.

Other than the above equations, inequality constraints may also be required. The most common ones are imposed upon the inlet and outlet concentrations, i.e.

$$C_{ik}^{\mathrm{in}} \le \beta_{ik} \qquad i \in \mathbf{U} \qquad k \in \mathbf{C} \tag{A6}$$

and

$$C_{ik}^{\mathrm{out}} \le \gamma_{ik} \qquad i \in \mathbf{U} \qquad k \in \mathbf{C} \tag{A7}$$

where β_{ik} and γ_{ik} denote respectively the maximum allowable concentrations of solute k at the inlet and outlet of unit i.

Water-Treatment Units. Only simple material balance equations are used in this work to model a general water-treatment unit. In particular, both water and solute balances should be considered, i.e.

$$F_j = \bar{F}_j + L_j \qquad j \in \mathbf{T} \tag{A8}$$

and

$$F_jC_{jk}^{\mathrm{in}} = M_{jk} + \bar{F}_jC_{jk}^{\mathrm{out}} + L_jD_{jk} \qquad j \in \mathbf{T} \qquad k \in \mathbf{C1} \tag{A9}$$

$$F_jC_{jk}^{\mathrm{in}} = F_jC_{jk}^{\mathrm{out}} \qquad j \in \mathbf{T} \qquad k \in \mathbf{C2} \tag{A10}$$

where F_j and $\bar{F}_j$ represent the water flow rates at the inlet and outlet of the water-treatment unit j, respectively, M_{jk} denotes the mass load in mass exchangers such as stripping, absorption, and solvent extraction, L_j denotes the corresponding water loss in operations such as evaporation, filtration, and membrane separation, etc., C_{jk}^{in} and C_{jk}^{out} are used to represent respectively the inlet and outlet concentrations of solute k, and D_{jk} is the concentration of solute k in the lost water. For unremovable solutes, $D_{jk} = 0$ and does not appear in eq A10.

An alternative expression of eq A8 is

$$L_j = \phi_jF_j \qquad j \in \mathbf{T} \tag{A11}$$

where ϕ_j is a design parameter that must be estimated beforehand. To characterize the performance of treatment units, two alternative models have been adopted. The first one is concerned with the removal ratio ψ_{jk}, i.e.

$$\frac{F_j C_{jk}^{\text{in}} - \bar{F}_j C_{jk}^{\text{out}}}{F_j C_{jk}^{\text{in}}} = \psi_{jk} \qquad j \in \mathbf{T} \qquad k \in \mathbf{C} \tag{A12}$$

where

$$1 > \psi_{jk} > 0 \qquad j \in \mathbf{T} \qquad k \in \mathbf{C1} \tag{A13}$$

$$\psi_{jk} = 0 \qquad j \in \mathbf{T} \qquad k \in \mathbf{C2} \tag{A14}$$

In the above equations, ψ_{jk} denotes the efficiency of removing solute k in unit j, and it is also considered to be a constant design parameter. The second model can be adopted if a process is believed to be equilibrium controlled, i.e.

$$C_{jk}^{\text{out}} = \lambda_{jk} \qquad j \in \mathbf{T} \qquad k \in \mathbf{C1} \tag{A15}$$

where λ_{jk} denotes the constant concentration of solute k achieved at the exit of unit j. Examples of these types of operations include stripping, extraction, evaporation, etc.

Additional inequality constraints are also necessary in certain cases. The most obvious one can be expressed in a form similar to eq A6, i.e.

$$C_{jk}^{\text{in}} \le \beta_{jk} \qquad j \in \mathbf{T} \qquad k \in \mathbf{C} \tag{A16}$$

Finally, in revamping applications, one may need to restrict the throughputs of certain units. This can be imposed with

$$F_j \le \eta_j \qquad j \in \mathbf{T} \tag{A17}$$

where η_j is the upper bound of the throughput in unit j.

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