Water Usage and Treatment Network Design Using Genetic Algorithms

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A mathematical programming model has been developed in this work to identify the cost-optimal and least-consumption water usage and treatment networks (WUTNs). The network configurations of WUTNs were generated on the basis of a superstructure embedded with the existing water-using units, the repeated water-treatment units, and the mixers. The benefits of using this model are clearly demonstrated in the examples. The genetic algorithms were used in this study to solve the WUTN optimization problem. Several techniques have been developed to enhance convergence in the evolution processes. First of all, by adopting the split fractions from splitting nodes as the design variables and devising an encoding strategy accordingly, the search space can be significantly reduced. Second, by cascading a series of evolution processes according to a set of "inducing" parameters, the appropriate ranges of the design variables can be efficiently determined. As a result, the need to obtain a good initial guess can be eliminated. The total number of generations to reach optimum can also be lowered to an acceptable level even for a large WUTN design problem.

Introduction

Sufficient water supply is essential for running any commercial chemical process. This is because water may be used in almost every phase of plant operation. In the process system, it may be considered not only as a reactant/product in reactors but also as a mass-separating agent (MSA) in separation processes such as absorption, extraction, leaching, and stripping. In the utility system, makeup water is constantly consumed in boilers and cooling towers. Further, it is also utilized for equipment cleaning, fire fighting, and other miscellaneous consumption. After these usages, wastewater streams are inevitably created. They should be treated/regenerated and then either reused/recycled within the plant boundary or discharged to the environment.

Although water is one of many abundant natural resources on earth, the demand for it has increased dramatically in the modern age due to rapid economic expansion in many regions worldwide. Consequently, there are real incentives to develop process integration methodologies with special emphasis on industrial water conservation. In the literature, there are only a few studies that address this problem specifically. Takama et al.[1] first proposed a nonlinear programming formulation to solve the water allocation problem in a refinery. In the works of Wang and Smith[2,3] and Kuo and Smith,[4,5] the design task was handled in two stages; i.e., the minimum process water consumption rate or wastewater treatment capacity was first determined according to a composite curve, and the network structure was then obtained manually based on heuristic procedures. Another alternative is to formulate the design problem of water usage and treatment networks (WUTNs) with the mass integration framework proposed by El-Halwagi et al.[6]

Since there are still drawbacks in the preliminary networks generated with the above methods, a mathematical programming model has been developed in a previous work[7] to finalize the optimal WUTN design. Although this approach was shown to be reliable, versatile, and more comprehensive, it is clear that further improvements can be incorporated into the model. Notice first that the process conditions of the water-using units in a WUTN are in general determined by the needs of chemical process. In other words, these units exist as a part of the process itself. On the other hand, as long as the environmental requirements can be satisfied, the network configuration for wastewater treatment and, further, the *number* of each type of unit used in the network are not limited. Thus, it may be beneficial to adopt several *repeated* water-treatment units in the same process. Second, it has been well recognized that the use of mixers can introduce additional flexibility in HEN design.[8] But none of the previous works took advantage of the additional opportunities created by merging and splitting water streams in the WUTN design.

The inclusion of these new features in WUTN inevitably increases the complexity of the mathematical programming model. Consequently, the effectiveness of solution techniques becomes a critical issue in the present study. The traditional gradient-based algorithms are notorious for their inability to avoid getting trapped in local optima. In addition, the convergence of numerical iteration procedure is highly dependent upon the location of the initial guess on the solution surface. Since these technical difficulties clearly make the conventional search methods less appealing, there is a need to look for an alternative approach to solve the modified WUTN design problem.

The genetic algorithms (GAs) can be considered as a stochastic evolution strategy imitating the natural selection process of biological species.[9,10] The basic analogy is established between a design parameter in the optimization problem and a *gene* in a *chromosome*

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(or individual). Thus, one chromosome represents a possible solution. A genetic algorithm takes a population of chromosomes and generates new populations according to a variety of evolution principles such as *reproduction*, *crossover*, and *mutation*. Each of these principles is only applicable to the chosen members of the population. The selection of these members is done randomly based on the *fitness* of each individual chromosome. This fitness measure is usually the objective function in an optimization problem. The constraint equations can often be handled by introducing additional penalty functions.

It is widely believed that the drawbacks of the gradient-based methods can be overcome by the use of genetic algorithms. In particular, the potential advantages of adopting GAs in the present study are as follows.

- The search result is not sensitive to the initial population.
- It is more likely to identify a global optimum.
- Multiple WUTN designs can be obtained for further evaluation.
- The design variables can be discrete.
- The derivatives of the objective function are not required.
- The algorithms can be implemented on parallel computers.

The objective of our study is thus to solve the modified WUTN design problem with genetic algorithms. The remainder of this paper is organized as follows. Since the original mathematical programming model has been modified, its formulation is first described briefly. Second, the implementation procedure is presented in detail. Two simple examples are presented in this paper to illustrate this procedure. Since the effects of incorporating mixers and *repeated* water-treatment units in WUTN can be easily studied with the proposed mathematical program, the benefits of such design practices are also clearly demonstrated in these examples. Finally, a case study involving the retrofit design of WUTN in a refinery is reported in detail at the end of this paper.

The Modified Mathematical Programming Model

To incorporate mixers and repeated treatment units in the WUTN design, it is necessary to revise the existing mathematical programming model[7] accordingly. In particular, the options to adopt these two types of units should be embedded in the superstructure and their unit models should be treated as additional constraint of the optimization problem. The unit model of mixers can be found in the Appendix. Notice that, although the models of the water-using units and water-treatment units have already been described in Huang et al.,[7] they are repeated in the same appendix for the sake of completeness.

Let us first introduce the definitions of three unit sets and a species set to facilitate concise formulation of the mathematical program, i.e.

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

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

$$\mathbf{X} = \{n | n \text{ is the label of a mixer in the plant; } n = 1, 2, ..., N_x\} \quad (3)$$

$$\mathbf{C} = \{k | k \text{ is the label of a solute in aqueous phase which affects water quality}\} \quad (4)$$

Water Sources and Sinks. Since 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.

(1) Primary Water. The most dependable sources of industrial water are those available in the environment. Once taken from the environment, these waters usually must go through a series of preliminary treatments before they can be consumed in various water-using units. To simplify our formulation, these preliminary treatment processes were not modeled explicitly. In the mathematical program, several primary water sources with different qualities have been adopted instead. Each one of them corresponds to a product of the preliminary treatment system and can be utilized in one or more water-using unit.

(2) Secondary Water. Other than the primary waters, it may be possible to find additional sources within the plant due to reaction and/or separation. Although these waters are usually of inferior quality, they are included to ensure the comprehensiveness of our optimization model.

On the basis of the present scope of optimization studies, all potential water sinks can be classified into three types.

(1) Type A. Wastewater can be discharged to the environment if its quality meets all requirements of government regulations. Several different destinations may be considered, e.g. soil, underground, river and sea, etc. Each imposes specific restrictions on the effluent.

(2) Type B. If the process plant is located in an industrial park, then there may be a common facility for treating the effluents from various plants on the site. In this case, this treatment system can also be regarded as a sink. Also, in revamping applications, it may be necessary to treat the existing central treatment process *within* the plant as a sink also.

(3) Type C. Operation losses are inevitable in certain water-using and water-treatment units. To account for material balance, these losses are sent to two fictitious exits of WUTN. One is used to collect all loss streams from the former units and the other is for the latter.

To achieve notational consistency, five sets of labels are defined on the basis of above classification:

$$\mathbf{I}_1 = \{p | p \text{ is the label of a primary source for WUTN; } p = 1, 2, ..., N_p\} \quad (5)$$

$$\mathbf{I}_2 = \{s | s \text{ is the label of a secondary source for WUTN; } s = 1, 2, ..., N_s\} \quad (6)$$

$$\mathbf{O}_A = \{a | a \text{ is the label of a Type A sink for WUTN; } a = 1, 2, ..., N_a\} \quad (7)$$

$$\mathbf{O}_B = \{b | b \text{ is the label of a Type B sink for WUTN; } b = 1, 2, ..., N_b\} \quad (8)$$

$$\mathbf{O}_C = \{c | c \text{ is the label of a Type C sink for WUTN; } c = U \text{ or } T\} \quad (9)$$

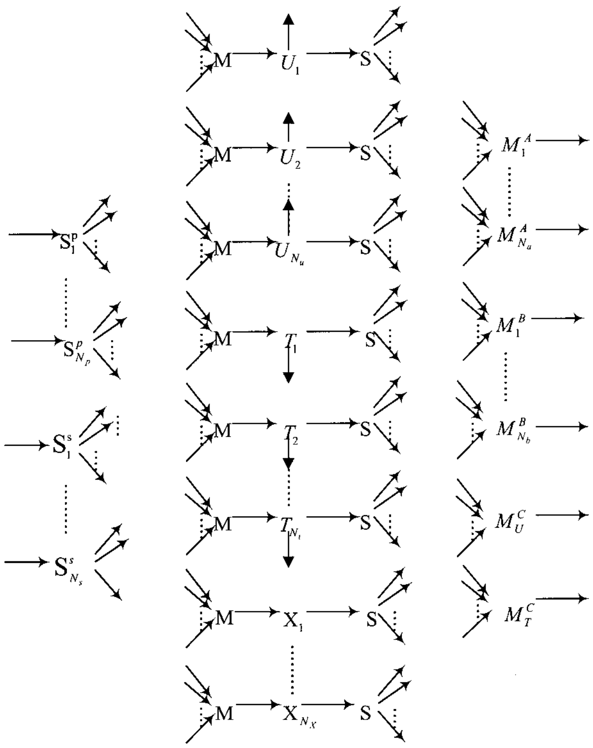

Figure 1. General superstructure for water usage and treatment networks.

The 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 a modified version of that suggested by Huang et al.[7] A simple construction procedure is presented below.

1. Place a mixing node at the inlet of every mixer, water-using unit and water-treatment unit.

2. Place a mixing node before each type A and each type B sink.

3. Place two mixing nodes to collect loss streams. The operation losses from all water-using units are connected to one and those from the water-treatment units are connected to the other.

4. Place a splitting node after each primary source. The split branches from every such node are connected to all the mixing nodes established in step 1.

5. Place a splitting node after each secondary source. The split branches from every such node are connected to all the mixing nodes established in steps 1 and 2.

6. Place a splitting node at the exit of every water-using and water-treatment unit. The split branches from every such node are connected to all the mixing nodes installed in steps 1 and 2 *except* the one before the same unit.

7. Place a splitting node at the exit of every mixer. The split branches from every such node are connected to all the mixing nodes established in step 1 *except* the one before itself.

This scheme can be represented by Figure 1, in which the symbol 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 types A and B; M_U^C and M_T^C denote the mixing nodes before type C sinks for water-using and water-treatment units respectively, $M - U_u - S$ ($u\in\mathbf{U}$) represents the uth water-using unit and the mixing and splitting nodes attached before and after this unit and, similarly, $M - T_t - S$ ($t\in\mathbf{T}$) and $M - X_x - S$ ($x\in\mathbf{X}$) represent respectively the tth water-treatment unit and the xth mixer with their attached mixing and splitting nodes. Notice that there is always one output from U_u or T_t which is not connected to the splitter on the exit. All such streams are connected to M_U^C or M_T^C.

The Mathematical Program. Having constructed the general stream structure for a given problem, an NLP model can then be formulated to determine the optimal WUTN. Notice that, other than the unit models described in the Appendix, the node models corresponding to all mixing and splitting nodes should also be included. More specifically, water and solute balances should be treated as constraint equations and, also, upper limits concerning wastewater flow rate and/or pollutant concentrations after the mixing points M_a^As and M_b^Bs must be imposed to satisfy environmental requirements at types A and B sinks. Finally, it is assumed that the solute concentrations in each primary and secondary source are given and the supply of every secondary water is limited.

Essentially two objective functions, F^C and F^W, have been considered in this study. The first is the overall operating cost of WUTN, i.e.

$$F^C = \sum_{u\in\mathbf{U}} \omega_u^X X_u + \sum_{t\in\mathbf{T}} \omega_t^Y Y_t + \sum_{b\in\mathbf{O}_B} \omega_b^Z Z_b^B \tag{10}$$

where Z_b^B is the discharge rate to the bth sink of type B. It is assumed in this work that the operating cost of a WUTN is dominated by those associated with running the water-using and water-treatment units and the treatment charges of type B sinks and, also, each expenditure is roughly proportional to the corresponding throughput. The weighting factors ω_u^X, ω_t^Y and ω_b^Z in the above function are used to reflect the relative costs associated with the uth water-using unit, the tth water-treatment unit and the bth sink of type B, respectively. It should be noted that a more appropriate network design can be obtained by incorporating both operating costs and capital costs in the objective function. However, since it is difficult to develop an accurate model in unified format to evaluate the capital costs of a wide variety of water-using and water-treatment units, it was our decision to adopt overall operating cost as the design objective in the present study for the sake of convenience and ease in computation.

From the standpoint of water conservation, one may also wish to synthesize a WUTN which utilizes the least amount of freshwater. In this case, the proper objective function is

$$F^W = \sum_{p\in\mathbf{I}_1} W_p^P \tag{11}$$

where W_p^P represents the consumption rate of the pth primary water. On the other hand, if the design objective is wastewater minimization, the performance of WUTN can obviously be measured with

$$F^W = \sum_{a\in\mathbf{O}_A} Z_a^A + \sum_{b\in\mathbf{O}_B} Z_b^B + (Z_U^C + Z_T^C) \tag{12}$$

where Z_a^A denotes the discharge rate to the ath sink of type A; Z_U^C and Z_T^C represent the combined flow rates of water losses from water-using units and water-treatment units, respectively. Notice that the above two design objectives, i.e., water conservation and wastewater minimization, can actually be achieved simultaneously with either eq 11 or eq 12. Thus, the latter is not considered throughout this paper.

Solution Procedure

To implement genetic algorithms, it is necessary to first devise a proper strategy to handle the constraint equations in the optimization problem. In principle, each of them can be satisfied in the evolution process eventually by designing a corresponding penalty function. However, this approach is often hampered by convergence difficulties. There is thus a need to develop a more practical method on the basis of a thorough analysis of the model structure.

A Unified Formulation of the Constraint Equations. The unit and node models in WUTN have already been described individually in the previous section. To facilitate the subsequent analysis, they are now rewritten with unified notation. In particular, the unit sets defined in eqs 1−3 can be combined, i.e.

$$\mathbf{P} = \mathbf{U} \cup \mathbf{T} \cup \mathbf{X} \quad (13)$$

Since, 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 their labels. In other words, the set of all splitting nodes can be defined as

$$\mathbf{S} = \mathbf{P} \cup \mathbf{I_1} \cup \mathbf{I_2} \quad (14)$$

Similarly, since 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

$$\mathbf{M} = \mathbf{P} \cup \mathbf{O_A} \cup \mathbf{O_B} \cup \mathbf{O_C} \quad (15)$$

The water balance around any splitting node can be written as

$$F_i^S = \sum_{j \in \mathbf{M}, j \neq i} f_{ij} \quad i \in \mathbf{S} \quad (16)$$

where F_i^S denotes the water flow rate from unit i to its downstream splitting node and f_{ij} represents the water flow rate from splitting node i to the mixing node j. Notice that the concentrations of each component before and after the splitting node remain unchanged.

The water balance around each mixing node can be expressed as

$$\sum_{n \in \mathbf{S}, n \neq m} f_{nm} = F_m^M \quad m \in \mathbf{M} \quad (17)$$

where F_m^M denotes the water flow rate entering unit m from its upstream mixing node. The corresponding component balance equation is

$$\sum_{n \in \mathbf{S}, n \neq m} f_{nm} C_{nk}^S = F_m^M C_{mk}^M \quad m \in \mathbf{M} \quad k \in \mathbf{C} \quad (18)$$

where C_{mk}^M is the concentration of solute k at the entrance of unit m and C_{nk}^S is the concentration of solute k at the exit of unit n.

From eqs A1, A2, A8, A10, and A15, it is clear that the water balance around a unit in $\mathbf{P}$ can be formulated in the following general form:

$$(1 - \rho_r) F_r^M = F_r^S \quad r \in \mathbf{P} \quad (19)$$

where ρ_r denotes the fraction of water loss in the incoming water of unit r.

Finally, it should be noted that the concentrations of solute k at the inlet and outlet of unit r, i.e., C_{rk}^M and C_{rk}^S, must satisfy additional balance equations, eqs A3, A9, and A16. If the water flow rates at the inlet and outlet of unit r can be regarded as *given information*, these three equations can be expressed in a unified format:

$$C_{rk}^M = a_r C_{rk}^S + b_r \quad r \in \mathbf{P} \quad k \in \mathbf{C} \quad (20)$$

where a_r and b_r are parameters which can be determined before solving the simultaneous component balance equations. In a large number of units, the amount of water loss is negligible and thus the last terms on the right side of eqs A3 and A9 can be removed. The mass load in eq A9 is a nonzero variable for units without water loss. In this situation, eq A11 can be used to express M_{jk} as a function of inlet concentration. On the other hand, if a loss stream does exist, the variable D_{ik}^X or D_{jk}^Y can be eliminated with eq A4 or A11. As a result, the component balance equations in the WUTN model can always be transformed into the general form given in eq 20 with the exception that the concentration of solute k at the exit of unit r is constant. In this case, eq 20 should be replaced with

$$C_{rk}^S = c_r \; r \in \mathbf{P} \quad k \in \mathbf{C} \quad (21)$$

where c_r is the parameter λ_{ik}^X given in eq A5 or λ_{jk}^Y in eq A12.

Selection of Design Variables. In solving a nonlinear programming program, selection of the independent design variables is a critical issue which must be settled before actually implementing the search algorithm. Generally speaking, in a system of N equations and M variables ($M \geq N$), a set of $M - N$ design variables can be readily identified with any of the available techniques, e.g. Stadtherr et al.[11] As long as their values are provided, the other M variables can be easily determined by solving the N equations. However, if these design variables are encoded according to their respective feasible ranges, the resulting values of the dependent variables may not be acceptable. In addition to the possibility of violating the inequality constraints imposed in the mathematical program, i.e., eqs A6, A7, A13, and A14, unreasonable physical parameters, e.g., negative flow rates and concentrations, may also be produced if the design variables are generated randomly. Although it is conceptually possible to eliminate the corresponding chromosomes by introducing penalty functions in the fitness measure, the convergence rate of the evolution process will be affected adversely. To enhance the solution efficiency, let us introduce a set of new variables, i.e., the *split factions* of branch streams from each splitting node, into the WUTN model. Specifically, eq 16 can be written as

$$f_{ij} = \Phi_{ij} F_i^S \quad i \in \mathbf{S} \quad j \in \mathbf{M} \quad (22)$$

where Φ_{ij} is the split fraction of the jth branch from splitting node i and $i \neq j$. The split fractions must satisfy additional constraints, i.e.

$$\sum_{j \in \mathbf{M}, j \neq i} \Phi_{ij} = 1 \quad i \in \mathbf{S} \tag{23}$$

By substituting eq 19 into eq 17, the water balance around each mixing node before a water-using or water-treatment unit can be written as

$$\frac{F_m^S}{1 - \rho_m} = \sum_{n \in \mathbf{S}, n \neq m} \Phi_{nm} F_n^S \quad m \in \mathbf{P} \tag{24}$$

If the consumption rates of primary waters and all the split fractions are given, eq 24 can be solved simultaneously to determine the flow rates of the output streams from all units and mixers in WUTN. The flow rate of any branch stream from split node i to mixing node j can then be calculated on the basis of eq 22. Finally, the flow rates of input streams to all units and mixers and the discharge rates to all sinks can be computed easily according to eq 17.

Once the flow rate of every stream in the superstructure is determined, the component balance equations of the mixers, water-using and water-treatment units can usually be expressed in the form of eq 20. Substituting eq 20 into eq 18 yields

$$\sum_{n \in \mathbf{S}, n \neq m} f_{nm} C_{nk}^S = F_m^M (a_m C_{mk}^S + b_m) \quad m \in \mathbf{P} \quad k \in \mathbf{C} \tag{25}$$

Since the solute concentrations in the primary and secondary waters should be considered as given information, these equations can be solved simultaneously to determine the concentration of component k at the outlet of every unit and every mixer in WUTN. The inlet concentrations can then be computed on the basis of eq 18. However, as mentioned previously, not all component balance equations can be written in the form of eq 20. If the outlet concentration of a unit is governed by eq A5 or eq A12, the corresponding equation in eq 25 should be replaced with eq 21. Since the resulting system is solvable, the concentration of every component in every stream of the superstructure can still be evaluated.

A flowchart of the above computation procedure is presented in Figure 2. We found that the improvements achieved by using the split fractions and the consumption rates of primary waters as the design variables are quite satisfactory. Not only can the possibilities of negative flow rates and concentrations be completely avoided in the evolution process, but also the search efficiency of genetic algorithms can be enhanced significantly.

Encoding Strategy. The first task in implementing the genetic algorithms is to encode the design variables. The traditional approach is to translate them into binary codes. However, for the sake of convenience and economy, the floating-point genes[12] are adopted in this study. In particular, instead of a binary number, each gene is represented with a real number g_{ij} between 0 and 1. As mentioned previously, the design variables used in this study can be classified into two types, i.e., the split fractions and the consumption rates of primary waters. In the former case, g_{ij} is associated with the branch stream from splitting node i to mixing node j.

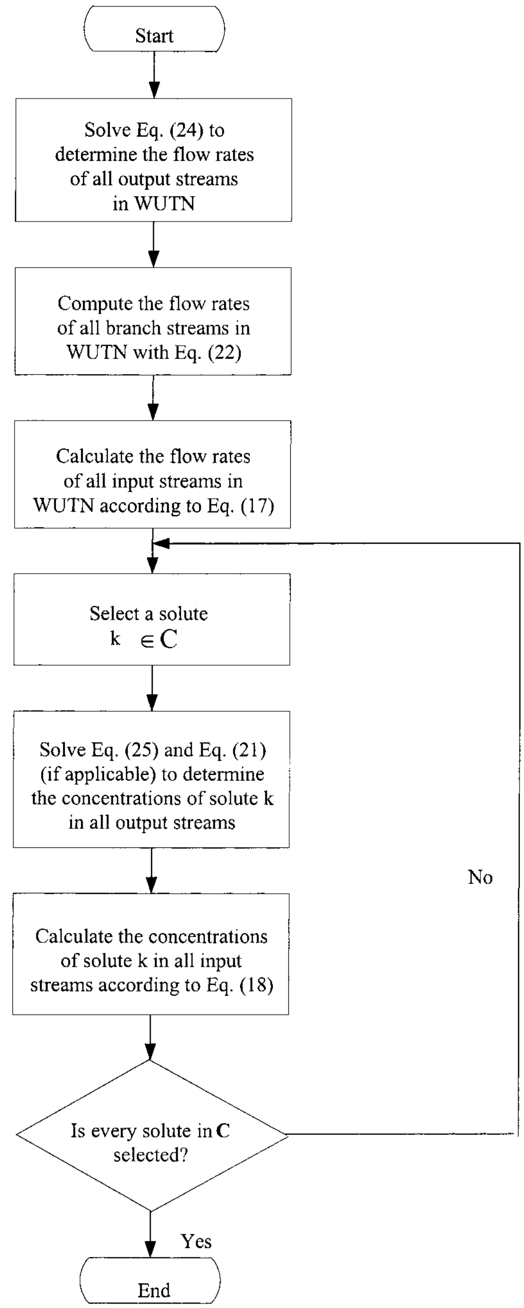

Figure 2. Solution procedure of water and component balance equations.

The split fractions can be computed according to

$$\Phi_{ij} = \frac{g_{ij}}{\sum_{l \in \mathbf{M}, l \neq i} g_{il}} \quad i \in \mathbf{S} \quad j \in \mathbf{M} \tag{25a}$$

where $i \neq j$. In the latter case, this number is mapped directly into the feasible range of the consumption rate of corresponding primary water. Thus, as long as these two types of floating-point codes are available, all the process variables in WUTN can be determined according to the flowchart presented in Figure 2.

Evolution Steps. The evolution process begins with an initial population. The genetic code of each chromosome in this population is produced with a random number generator. Once the initial population is available, three commonly used evolution steps, i.e., reproduction, crossover, and mutation, are followed repeatedly until the total number of generations reaches an assigned value. In this study, the reproduction step is done according to the popular roulette-wheel selection scheme. A two-point crossover procedure is then implemented to swap genes between chromosomes. Finally, the uniform mutation technique is adopted to alter the genetic codes of several randomly chosen chromosomes. Since these steps are well documented in the literature, e.g., see Michalewicz,[10] the detailed descriptions of these algorithms are omitted in this paper for the sake of brevity.

After reproduction, crossover and mutation are performed in each generation, an elitism strategy is practiced to preserve the best chromosome identified so far. In particular, the largest fitness value achieved in the current generation is compared with that of a chromosome temporarily stored in a buffer. If the former is larger, then this chromosome should be stored instead and the current population remains unchanged. Otherwise, the worst chromosome in the current population should be replaced by the one originally stored in the buffer.

Fitness Function. To facilitate implementation of the roulette-wheel selection scheme in reproduction, the fitness measure must always be represented with a positive number. On the other hand, the objective functions adopted in the WUTN design problem, i.e., the operating cost and freshwater consumption rate, should be minimized. Thus, a fitness function *fit* has been designed to incorporate these considerations in the evolution procedure:

$$fit(\mathbf{y}) = \frac{const}{obj(\mathbf{y}) + \sum_i wt_i pen_i(y_i) + res} \qquad (26)$$

where **y** is the vector of all process variables in the constraint equations; *obj* denotes the objective function of optimization problem; pen_i represents the penalty function associated with the *i*th inequality constraint and wt_i is the corresponding weight; *const* and *res* are two arbitrarily chosen positive constants. The objective functions used in this study has already been described previously in eqs 10 and 11. The penalty functions can be expressed as

$$pen_i(y_i) = \begin{cases} (y_i - U_i)^2 & \text{if } y_i > U_i \\ (L_i - y_i)^2 & \text{if } L_i > y_i \\ 0 & \text{otherwise} \end{cases} \qquad (27)$$

where U_i and L_i denote respectively the upper and lower limits of the *i*th process variable.

Inducing Mechanism. Since the number of process variables in a WUTN model is very large, the search efficiency of GAs for the present optimization problem is in general not satisfactory. A cascade evolution strategy is thus proposed to alleviate the convergence problem. In particular, a set of *inducing parameters* d_{ij} are introduced in computing the split ratios, i.e.

$$\Phi_{ij} = \frac{d_{ij} g_{ij}}{\sum_{n \in \mathbf{M}, n \neq i} d_{in} g_{in}} \quad i \in \mathbf{S} \quad j \in \mathbf{M} \qquad (28)$$

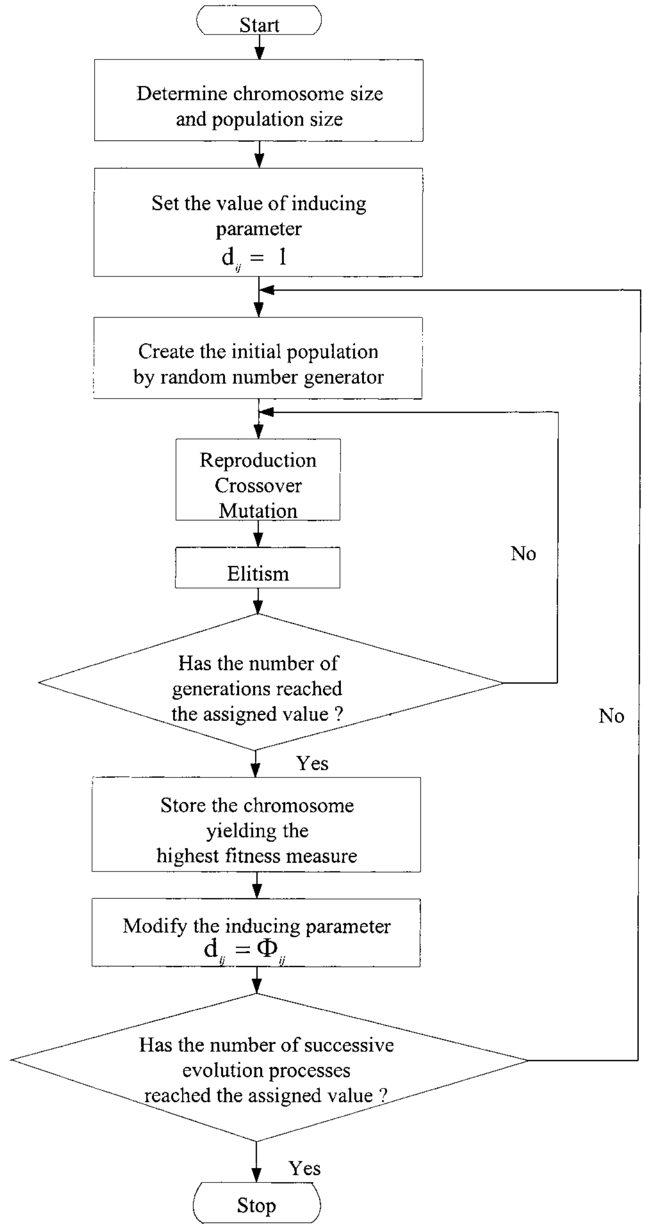

Figure 3. Cascade evolution procedure.

A series of evolution processes can be carried out in sequence. The values of these inducing parameters are set to one in the initial evolution process. The inducing parameters in the subsequent processes are reset according to the best chromosome identified in the previous process, i.e.

$$d_{ij}^{(k)} = \Phi_{ij}^{(k-1)} \quad i \in \mathbf{S} \quad j \in \mathbf{M} \qquad (29)$$

where $d_{ij}^{(k)}$ denotes the inducing parameter used in the *k*th evolution process, $\Phi_{ij}^{(k-1)}$ represents the split fraction identified from the best chromosome in the $(k - 1)$th process and $k = 1, 2, ...$ A flowchart of this cascade evolution procedure is presented in Figure 3.

Simple Examples

Two fictitious examples are presented here to illustrate the implementation procedure and to demonstrate the advantages of our approach.

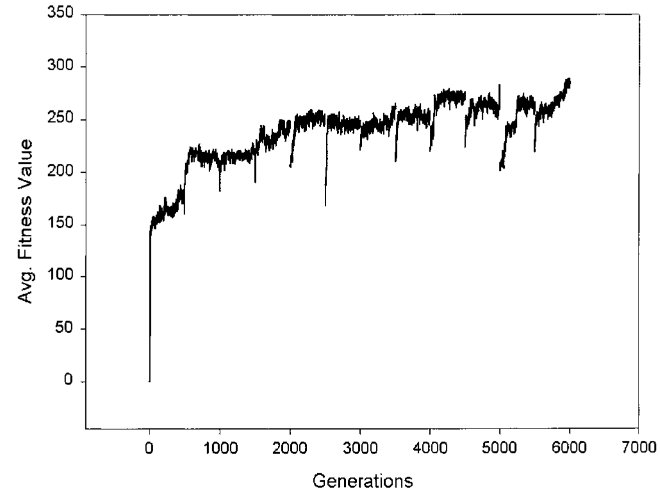

Figure 4. Average fitness measure of case 1 in example 1.

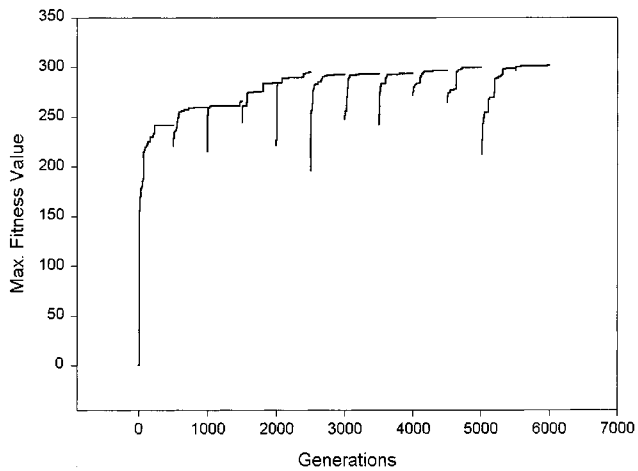

Figure 5. Best fitness measure of case 1 in example 1.

Table 1. Water Sources of Example 1

source no.	concn (ppm) solute A	solute B	max. flow rate (tons/h)
W_1	10	20	∞
W_2	600	300	50

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

unit no. (U_i)	solute (k)	mass load μ_{ik} (kg/h)	max. inlet concn β_{ik}^X (ppm)	max. outlet concn γ_{ik}^X (ppm)
U_1	A	10	200	600
	B	5	100	300
U_2	A	2	40	120
	B	8	120	360

Example 1. Consider a fictitious process with two water sources and one sink. Let us assume that there are two key solutes (A and B) in its water network that may cause environmental concerns. The properties of the sources are listed in Table 1. Notice that primary water is available only from the first source. Also, due to government regulations, the concentrations of both solutes in the wastewater must be lowered to at least 75 ppm before discharge to the environment. The process data of existing water-using units can be found in Table 2. Notice that these units can be described with eqs A1 and A3 under the condition that $\nu_1 = \nu_2 = 0$. The process data of the available water-treatment units are given in Table 3. Notice that these two treatment units are modeled according to eqs A8–A11 and, also,

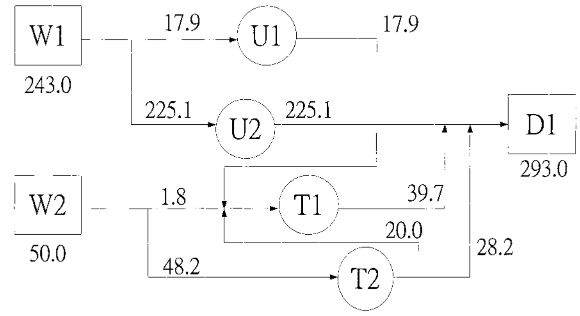

Figure 6. WUTN structure of a cost-optimal design for example 1. Case 1: The superstructure does not contain mixers and repeated units.

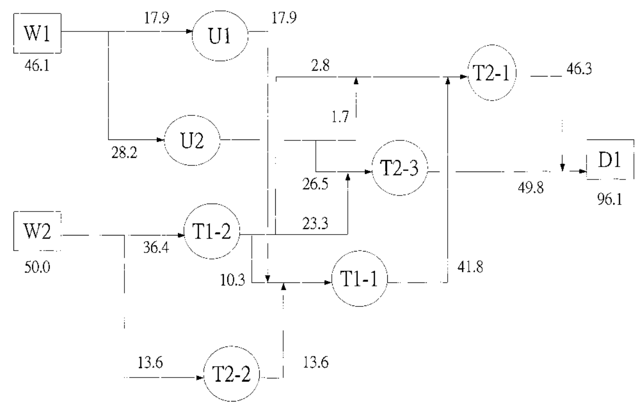

Figure 7. WUTN structure of a cost-optimal design for example 1. Case 2: There are three T_1 and three T_2 in the superstructure.

Table 3. Process Data of Water-Treatment Units in Example 1

unit no. (T_j)	solute (k)	removal ratio ψ_{jk}	max. throughput η_j (tons/h)
1	A	0.8	50
	B	0.1	
2	A	0.2	50
	B	0.7	

Table 4. GA Parameters in Cascade Evolution Processes of Example 1

GA parameter	value
population size	100
resolution	10 000
crossover rate	0.85
mutation rate	0.05
fitness constant—*const*	100000.0
fitness constant—*res*	1.0
no. of successive evolution processes	12
no. of generations in each process	500

none of these operations result in water loss; i.e. $\phi_1 = \phi_2 = 0$. In the present example, the minimum-cost WUTNs are generated according to the objective function F^C defined in eq 10 with equal weighting factors. Finally, the GA parameters used in all cascade evolution processes of this example can be found in Table 4. The crossover rate and mutation rate in this table were chosen according to the suggestions of Dorsey and Mayer[13] and the other parameters were tuned on a trial-and-error basis.

Let us first try to synthesize an optimal WUTN without the mixers and repeated water-treatment units. In other words, the superstructure contains only the two water-using units listed in Table 2 and the two water-treatment units listed in Table 3. After constructing the unit and node models, the design variables can be

Table 5. Operating Conditions of Process Units in the Cost-Optimal WUTN for Example 1, Case 1: One T_1 and One T_2

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U_1	17.9	A	10.0	568.9
		B	20.0	299.5
U_2	225.1	A	10.0	18.9
		B	20.0	55.5
T_1	39.7	A	525.6	105.1
		B	194.0	174.6
T_2	48.2	A	600.0	480.0
		B	300.0	90.0

identified and the chromosomes can then be encoded accordingly. The length of each chromosome in this case was found to be 32. The resulting mathematical program was solved on the basis of the flowchart presented in Figure 3. The average and best fitness measures of each generation in the cascade evolution processes are plotted in Figures 4 and 5, respectively. Since the initial population in each of the 12 successive processes was generated randomly, it can be observed that the average and best values of corresponding fitness measure drops periodically. However, it is also clear that this value tends to grow from generation to generation in each process and the best values in the last several processes reach an almost stable level. It should be noted that the search results appear to be unsatisfactory in the first three processes. This is due to the facts that the values of design variables are unknown initially and thus the feasible ranges stipulated in the search algorithm are often too wide. As a result, the probability of producing poor initial guesses becomes very high. This situation can be improved gradually by adjusting the inducing parameters (see Figures 4 and 5). This convergence-inducing capability is significant in the sense that the success of search does not rely on fair initialization, which is a common requirement of the other iterative optimization techniques. The resulting network configuration is presented in Figure 6. The flow rates and inlet and outlet concentrations of all water-using and water-treatment units in this network are listed in Table 5. The total capacity associated with the fittest chromosome in this case is 330.8 tons/h.

Next, let us evaluate the effects of adding repeated units in WUTN design. Specifically, two sets of identical treatment units, i.e., three T_1s and three T_2s, are introduced into the superstructure. The resulting cost-optimal WUTN is presented in Figure 7, and the corresponding process data are listed in Table 6. Notice that the third T_1 is bypassed in the final design. When compared with the original results, one can find that the total capacity is significantly reduced to 234.0 tons/h.

Example 2. An alternative design emphasis is adopted in this example, i.e., water conservation (or waste minimization). Thus, the optimal WUTN configuration in this case should be identified according to the objective function F^W defined in eq 11. The properties of three water sources considered here are listed in Table 7. 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 A and B are both 10 ppm. The process data of three existing water-using units in WUTN are presented in Table 8 and eqs A1, A3, A6, and A7 can be used to formulate the corresponding unit models. In the case of U_1 and U_2, the mass loads are specified and $\nu_1 = \nu_2 = 0$. On the other hand, there is a water loss of 15 tons/h

Table 6. Operating Conditions of Process Units in the Cost-Optimal WUTN for Example 1, Case 2: Three T_1 and Three T_2

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U_1	17.9	A	10.0	569.2
		B	20.0	299.6
U_2	28.2	A	10.0	80.8
		B	20.0	303.3
$T_1 - 1$	41.8	A	429.2	85.8
		B	224.2	201.7
$T_1 - 2$	36.4	A	600.0	120.0
		B	300.0	270.0
$T_2 - 1$	46.3	A	87.6	70.1
		B	209.4	62.8
$T_2 - 2$	13.6	A	600.0	480.0
		B	300.0	90.0
$T_2 - 3$	49.8	A	99.1	79.3
		B	287.7	86.3

Table 7. Water Sources of Example 2

	concentration (ppm)		
source no.	solute A	solute B	max. flow rate (tons/h)
W_1	0.1	0.1	∞
W_2	60.0	28.0	30.0
W_3	1800.0	1200.0	40.0

Table 8. Process Data of Water-Using Units in Example 2

unit no. (U_i)	solute (k)	mass load μ_{ik} (kg/h)	max. inlet concn β^X_{ik} (ppm)	max. outlet concn γ^X_{ik} (ppm)	water loss ν_i (tons/h)
U_1	A	8.0	0.1	100.4	0
	B	4.0	25.0	75.0	
U_2	A	11.2	80.0	240.0	0
	B	4.2	30.0	90.0	
U_3	A	0.0	8.0	8.0	15.0
	B	0.0	5.0	5.0	

Table 9. Process Data of Water-Treatment Units in Example 2

unit no. (T_j)	solute (k)	removal ratio ψ_{jk}	max. inlet concn β^Y_{jk} (ppm)	const outlet concn λ^Y_{jk} (ppm)	max. throughput η_j (tons/h)
T_1	A	0.9			125.0
	B	0.1			
T_2	A	0.2			125.0
	B	0.95			
T_3	A		200.0	5.0	125.0
	B		100.0	5.0	

in the third unit U_3 and thus two additional constraints, i.e., eq A4, should be imposed upon the solute concentrations in the loss stream. The process data of three available water-treatment units are given in Table 9. These units can be described with eqs A8–A10 and A14. 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 T_1 and T_2 are specified in Table 9. Thus, the four additional equations associated with eq A11 should be included in the mathematical program. Notice also that the exit concentrations of T_3 are assumed to be constant in this example. The two corresponding constraints should be formulated according to eq A12.

The least-consumption WUTN was first generated by using a superstructure without the mixers and repeated water treatment units. A mathematical program can be formulated accordingly. The design variables were identified and encoded into chromosomes of length 54. The GA parameters used in this example are the same as those in example 1 (see Table 4). The solution of this NLP problem is presented in Figure 8 and Table 10.

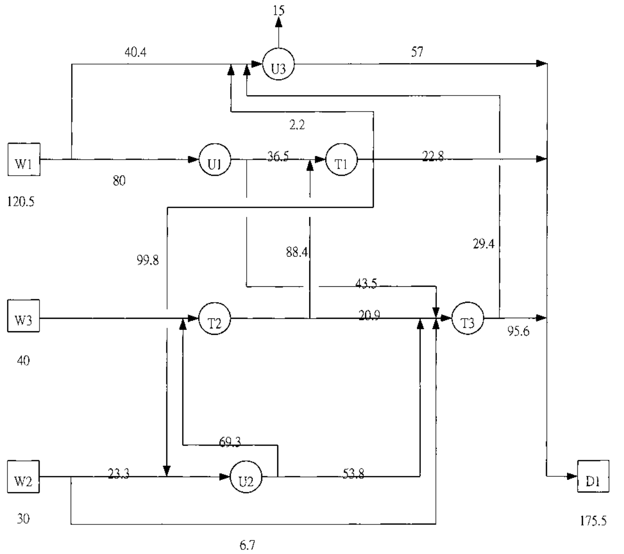

Figure 8. WUTN structure of a least-consumption design for example 2. Case 1: The superstructure does not contain mixers and repeated units.

Table 10. Operating Conditions of Process Units in the Least-Consumption WUTN for Example 2

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U_1	80.0	A	0.1	100.1
		B	0.1	50.1
U_2	123.2	A	48.0	138.9
		B	28.3	62.4
U_3	72.0	A	3.5	4.4
		B	3.0	3.8
T_1	124.9	A	452.0	45.2
		B	31.6	28.4
T_2	109.3	A	746.7	597.4
		B	478.7	23.9
T_3	124.9	A	198.0	5.0
		B	49.9	5.0

The minimum freshwater consumption rate in this case was found to be 120.5 tons/h. The discharge concentrations of solutes A and B were 10.0 and 7.6 ppm respectively.

Next, the impacts of mixers and repeated treatment units were studied. In the former case, three mixers were added in the superstructure. The minimum consumption rate of freshwater in the corresponding WUTN was reduced to 118.7 tons/h. In the latter case, four T_1s, four T_2s, and three T_3s were introduced into the superstructure. Since the solute-removal capability of the WUTN was greatly enhanced by including these additional treatment units, the solution showed that the requirement of freshwater could be eliminated entirely.

For comparison purpose, the original superstructure, i.e., the one without mixers and repeated units, was used again to synthesize a cost-optimal WUTN on the basis of objective function F^C. The resulting network configuration can be found in Figure 9. The detailed process conditions of all units in this network are presented in Table 11. The values of objective functions F^C and F^W associated with the cost-optimal network and the least-consumption network are summarized in Table 12. From these results, one can see that the two design objectives are not entirely compatible. If one tries to minimize the operating cost of WUTN, the resulting consumption rate of freshwater will be higher than that needed in the design obtained with objective function F^W. However, a larger-than-minimum total capacity will always be required if one tries to reduce the use of freshwater in the minimum-cost WUTN. In the former case, a simple structure is in general preferred in WUTN design. The needs of U_1 and U_3 are satisfied with primary water since the water-quality requirements of these two units are significantly more stringent than those of U_2. All treated waters are basically discharged to the environment. On the other hand, the network structure in the latter case tends to be more complex. One obvious feature is its recycle streams, i.e., the regenerated waters are utilized as much as possible. This is apparently an effective means of reducing freshwater consumption.

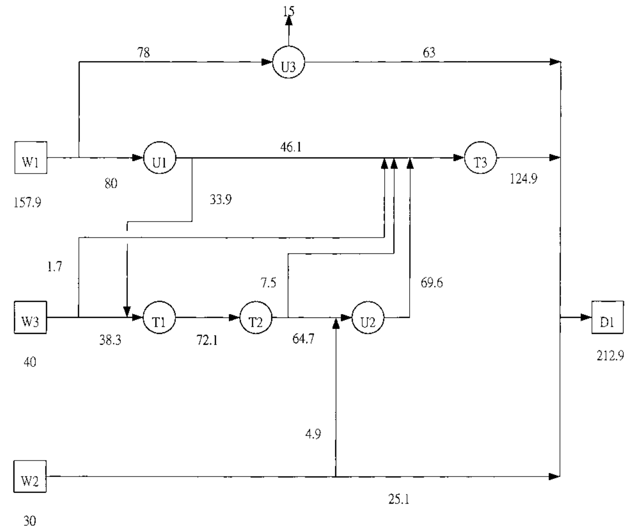

Figure 9. WUTN structure of a cost-optimal design for example 2. Case 4: The superstructure does not contain mixers and repeated units.

Table 11. Operating Conditions of Process Units in the Cost-Optimal WUTN for Example 2

process unit	throughput (tons/h)	solute	inlet concn (ppm)	outlet concn (ppm)
U_1	80.0	A	0.1	100.1
		B	0.1	50.1
U_2	69.6	A	78.8	239.7
		B	29.6	90.0
U_3	78.0	A	0.1	0.124
		B	0.1	0.124
T_1	72.1	A	1002.3	100.2
		B	660.4	594.4
T_2	72.1	A	100.2	80.24
		B	594.4	29.7
T_3	124.9	A	200.0	5.0
		B	86.8	5.0

Table 12. Comparison between the Cost-Optimal and Least-Consumption Designs in Example 2

design objective	F^C	F^W
minimum operating cost	496.7	157.9
minimum freshwater consumption	634.3	120.5

Case Study

The proposed procedure has been applied to a realistic problem concerning the retrofit of WUTN in a refinery. This problem was first discussed in an earlier study.[7] For the sake of brevity, the detailed process description is omitted in this paper. Instead, a simplified block diagram of the original process is presented in Figure 10.

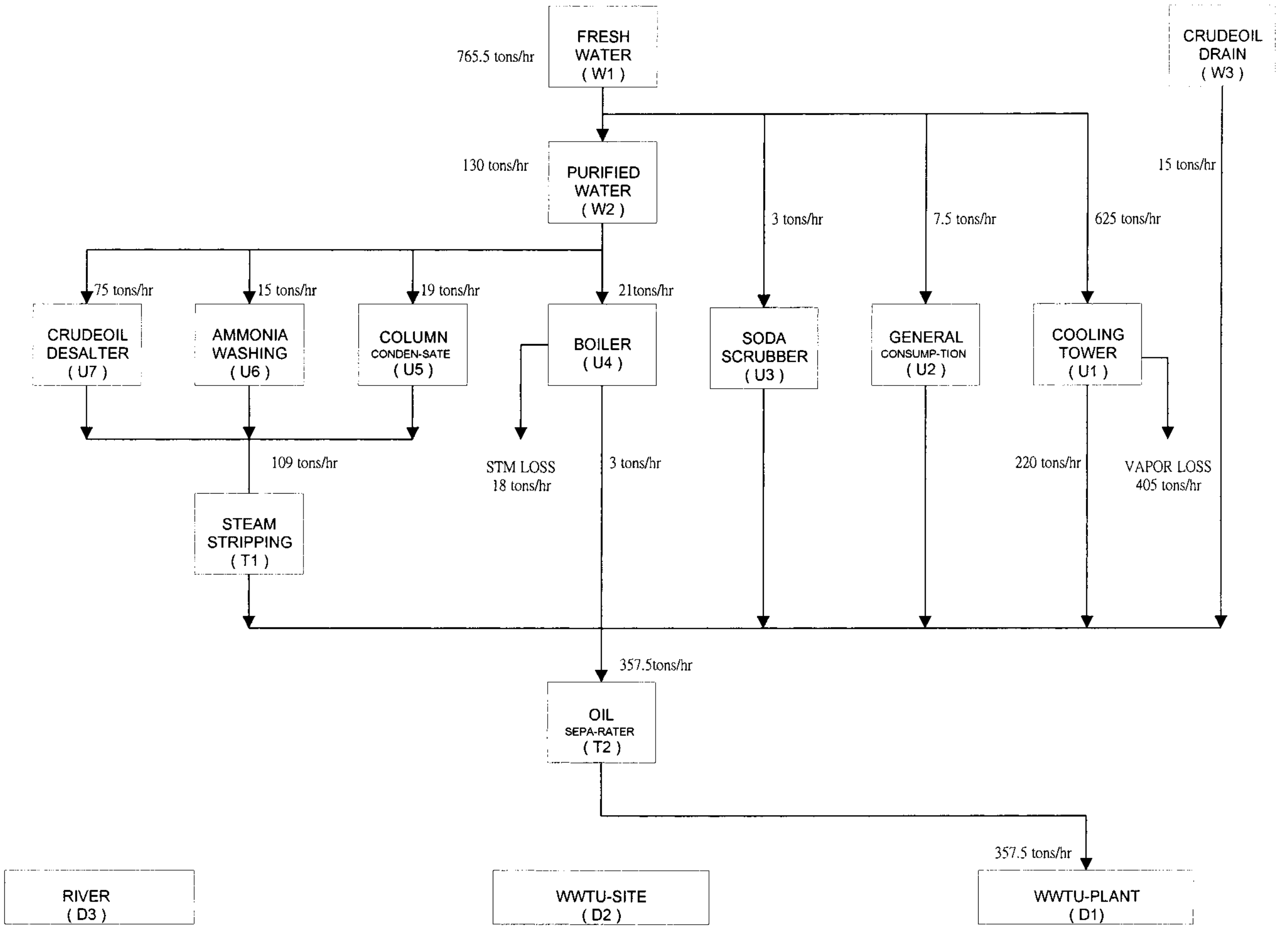

Figure 10. Block diagram of original WUTN in the refinery.

Table 13. Water Sources of the Refinery

water source	concentration (ppm) salts	organics	H_2S	max. flow rate (tons/h)
fresh water (W_1)	50	15	0	∞
purified water (W_2)	10	1	0	∞
crude drain (W_3)	135	45	400	15

Table 14. Water Sinks of the Refinery

water sinks	max. concn (ppm) salts	organics	H_2S	max. flow rate (tons/h)
WWTU (plant) (D_1)	364	759	24	360
WWTU (site) (D_2)	300	600	20	200
river (D_3)	50	200	10	∞

The properties of all available water sources are summarized in Table 13. In the present application, there are three possible options for discharging the wastewater. The process data of these water sinks are provided in Table 14. The acronyms WWTU(plant) and WWTU(site) represent the centralized wastewater treatment units in plant and on site, respectively.

The process data of all water-using units considered in this case study are summarized in Table 15. Notice that no significant water loss occurs in any of these units except U_1 and U_4. The flow rates of loss streams can be determined according to eq A2 and the water-loss fractions θ_1 and θ_4. The concentrations of inorganic salts and H_2S are assumed to be negligible in the lost streams of these two units, i.e., eq A4 is applicable here. On the other hand, the concentrations of organics at the exits of units U_1 and U_4 are assumed to be constant. In other words, eq A5 is adopted in these situations and the values of λ_{ik}^Xs are marked with asterisks in the table.

Table 15. Process Data of Existing Water-Using Units in the Refinery

unit no. (U_i)	solute (k)	μ_{ik} (kg/h)	β_{ik}^X (ppm)	γ_{ik}^X (ppm)	θ_i
cooling	salts	0	2500	3115	
tower	organics	0	220	220*	0.65
(U_1)	H_2S	0	45	45	
general	salts	7.125	300		
consumption	organics	52.5	50		0.0
(U_2)	H_2S	0.221	0		
soda	salts	0.18	300	500	
scrubber	organics	1.2	50	500	0.0
(U_3)	H_2S	1.75	5000	12 500	
steam	salts	0	10	150	
boiler	organics	0	1	50*	0.85
(U_4)	H_2S	0	0	0	
fractionation	salts	3.61	10	200	
column	organics	104.481	1	6500	0.0
(U_5)	H_2S	2.5	0	500	
ammonia	salts	7.485	10	7500	
wash	organics	81.75	50	6500	0.0
(U_6)	H_2S	3.2	50	480	
crude	salts	120.0	200	9500	
desalter	organics	480.0	100	6500	0.0
(U_7)	H_2S	1.875	20	45	

The process data of two existing water-treatment units can be found in Table 16. Notice that eqs A8−A11 and A14 are adopted to describe both units, and there are no water losses; i.e., $\phi_1 = \phi_2 = 0$. Also, no limitations are imposed on the inlet concentrations.

Table 16. Process Data of Existing Water-Treatment Units in the Refinery

unit no. (T_j)	solute (k)	ψ_{jk}	η_j (tons/h)
steam stripper (T_1)	salts	0	
	organics	0.25	150
	H_2S	0.95	
API separator (T_2)	salts	0.25	
	organics	0.55	400
	H_2S	0	

The objective functions considered in the present study are the same as those in the two simple examples discussed in the previous section, i.e., F^C and F^W. In the former case, since the operating cost of WWTU(plant) was considered by the plant personnel to be higher than those of WWTU(site) and also other units in WUTN roughly by a factor of 2, thus a value of 2 was assigned to the weighting factor associated with the sink representing WWTU(plant), i.e., $\omega_1^Z = 2.0$, and all other weighting factors in F^C were set to be one. On the basis of the data given in Figure 10, the values of F^W and F^C were determined to be 1947 and 765.5, respectively.

To address other practical concerns in plant operation, additional constraints have be included in the formulation for WUTN synthesis. In particular, the following points are made.

• It is believed that the makeup water in cooling tower (U_1) should be kept above 405 tons/h due to evaporation and blow-down. Also, a minimum water-consumption level, i.e., 7.5 t/h, should always be maintained for general use (U_2).

• Because of the requirement for high-quality water, each of the mixing nodes before units U_4 (steam generation), U_5 (ammonia wash), and U_6 (fractionation) is connected with a branch from the splitting node for purified water *only*.

• Since the API separator may receive wastewaters from various other origins, the treated water is generally considered to be not suitable for reuse. Thus, a conservative design can be obtained by eliminating the branches between the splitting node after T_2 and the mixing nodes before all water-using units.

By adding those constraints, the mathematical program can be formulated on the basis of a superstructure. The superstructure for retrofitting purpose should contain only the existing units listed in Tables 15 and 16. The first one considered in this study was built without mixers. The corresponding optimization problems were then solved with genetic algorithms according to the proposed procedure. The GA parameters listed in Table 4 were again used in the evolution processes. The length of each chromosome in this case was set to be 137.

The resulting cost-optimal design is presented in in Figure 11. It should be noted that the operating cost of this design is lower than that of the current practice. A 12.5% reduction in F^C, i.e., from 1947 to 1704, can be achieved simply by rearranging the WUTN configuration. From Figure 11, one can observe that the handling of drainwater from the crude oil (W_3) is different from that in the original design. Since the charge of sink D_1 is higher, a portion of the wastewater is sent to D_2 after treatment in the water-treatment units and/or mixing with other streams. Also, due to more stringent requirements in water quality, the waters consumed in U_4 (steam boiler), U_5 (fractionation column), and U_6 (ammonia wash) are supplied with the second source W_2, i.e., the purified water. On the other hand, the freshwater (W_1) is good enough for general use (U_2) and desalter (U_7). Notice that part of the water used in cooling tower U_1 is taken from other water-using units, i.e., U_5 and U_7. This is because of the fact the relatively high impurity concentrations can be tolerated in operating a cooling tower. The waters from the water-using units are in general first treated in the water-treatment units T_1 and T_2 and then sent to D_1 and D_2 for final treatment. Since the waters from U_2, U_3, and U_5 are cleaner, their split streams can be combined and discharged to the environment (D_3) directly.

The least-consumption WUTN is presented in Figure 12. In this case, a saving of 18.2% (from 765.5 to 625.9 tons/h) in freshwater can be achieved. There are two distinctive features in the network configuration. First of all, to minimize the water usage of WUTN, it is highly desirable to promote regeneration, reuse, and recycling without discharging wastewaters to the sinks. Also, the wastewaters are all discharged to D_1 and D_2 since their requirements are not as strict as those of the river (D_3) and cost is not our emphasis in the present design.

If more complex network structures are acceptable, then mixers can be introduced into the superstructure. In our study, three were adopted and consequently the length of each chromosome was increased to 205. The resulting least-consumption network can be found in Figure 13. The freshwater consumption rate in this case is now lowered to 594.2 tons/h, which represents a 22.4% reduction from its original level.

Conclusions

A mathematical programming model is developed in this work to identify the cost-optimal and least-consumption WUTNs. In addition to the water-using units, the mixers and the repeated water-treatment units are introduced in the proposed superstructure to incorporate a high level of flexibility in design. The benefits of such a strategy are clearly demonstrated in the simple examples. This mathematical program has also been utilized in the case studies for retrofitting the water distribution system in a refinery. The resulting improvements are quite satisfactory.

The genetic algorithms were used to solve the WUTN optimization problem. Several techniques have been developed to enhance convergence in the evolution processes. In particular,

• By adopting the split fractions as design variables and the encoding strategy define in eq 25, the search space can be significantly reduced.

• By cascading the evolution processes according to the inducing parameters, the appropriate ranges of the design variables can be efficiently determined.

As a result, there is no need to obtain a good initial guess to ensure reasonable solution. The total number of generations to reach optimum can also be decreased to an acceptable level even for a large WUTN design problem.

Acknowledgment

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Appendix: The Unit Models

The equipments considered in the present study are divided into three categories, i.e., water-using units,

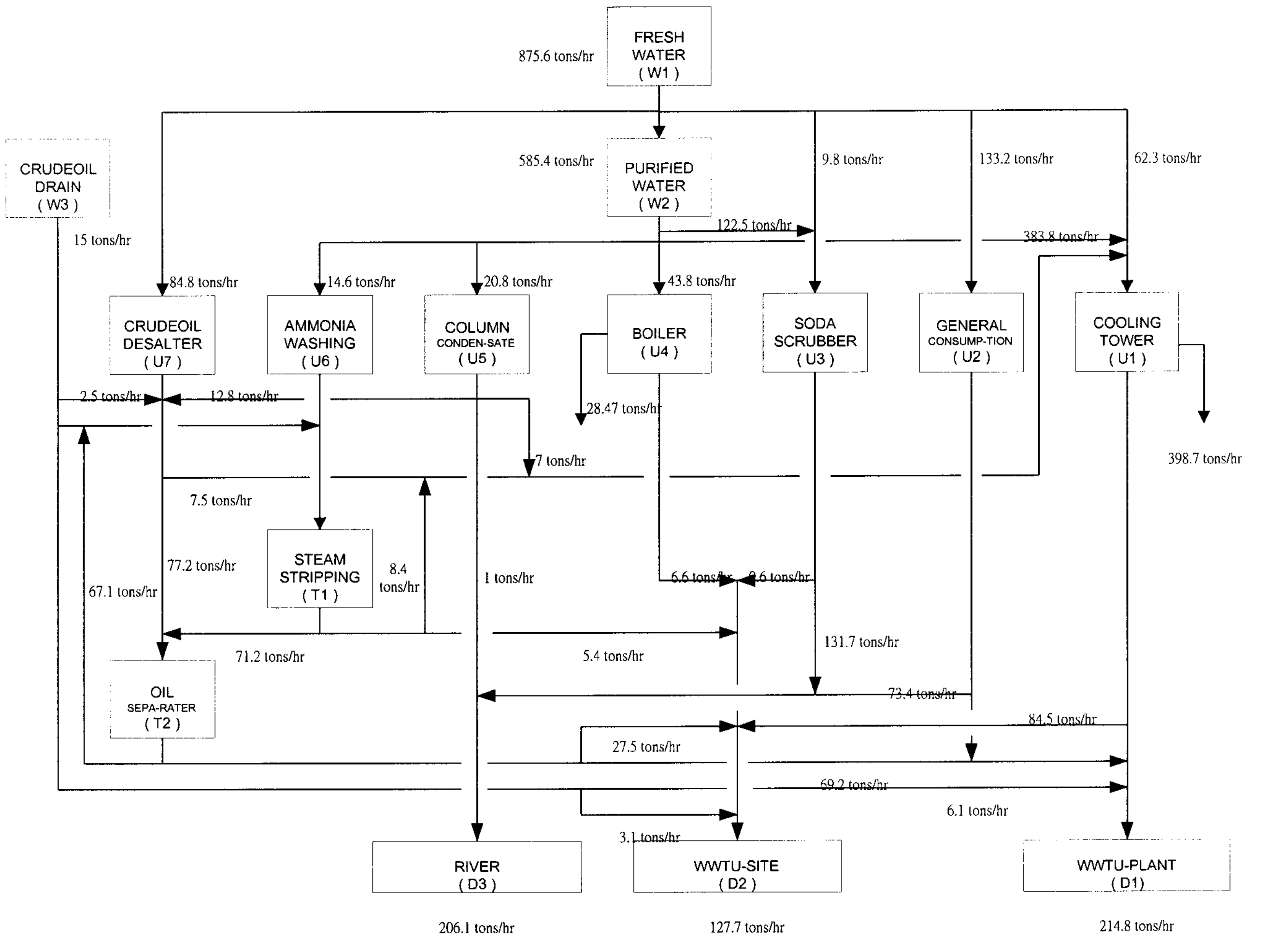

Figure 11. Block diagram of a cost-optimal WUTN in the refinery. Case 1: The superstructure does not contain mixers and repeated units.

water-treatment units and mixers. 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:

The 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

$$X_i = \bar{X}_i + \nu_i \quad i \in \mathbf{U} \tag{A1}$$

where X_i and $\bar{X}_i$ denote respectively the water flow rates at the inlet and outlet of unit i, and ν_i is the operation loss. Notice that $\nu_i = 0$ in almost all mass exchangers and in reactors where water is an inert. On the other hand, ν_i is positive in steam generators, cooling towers and reactors where water is a consumed. In the case of nonzero water loss, ν_i becomes a design parameter which must be determined according to operating conditions of the unit before solving the mathematical program. An alternative formulation of eq A1 can be written as

$$(1 - \theta_1)X_i = \bar{X}_i \quad i \in \mathbf{U} \tag{A2}$$

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 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.

$$X_i B_{ik}^X + \mu_{ik} = \bar{X}_i C_{ik}^X + \nu_i D_{ik}^X \quad i \in \mathbf{U} \quad k \in \mathbf{S} \tag{A3}$$

where B_{ik}^X and C_{ik}^X represent respectively the concentrations of solute k at the inlet and outlet of the water-using unit i, D_{ik}^X is the concentration of solute k in the loss stream, and μ_{ik} is the mass load of solute k in unit i. In the case of reaction, μ_{ik} can be negative, zero, or positive depending on whether solute k is a reactant, an inert material, or a product. It is assumed in this study that, in each mass exchanger that utilized water as MSA, the mass load μ_{ik} is positive and can be considered as a given design parameter. In other words, we assume that the flow rate of rich stream and its inlet and outlet concentrations have already been determined in advance by some other means. Notice also that μ_{ik} should be zero in all utility generation units.

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.

$$D_{ik}^X = 0 \quad i \in \mathbf{U} \quad k \in \mathbf{S} \tag{A4}$$

For example, the amount of nonvolatile inorganics in the leaked steam is indeed negligible. In other situa-

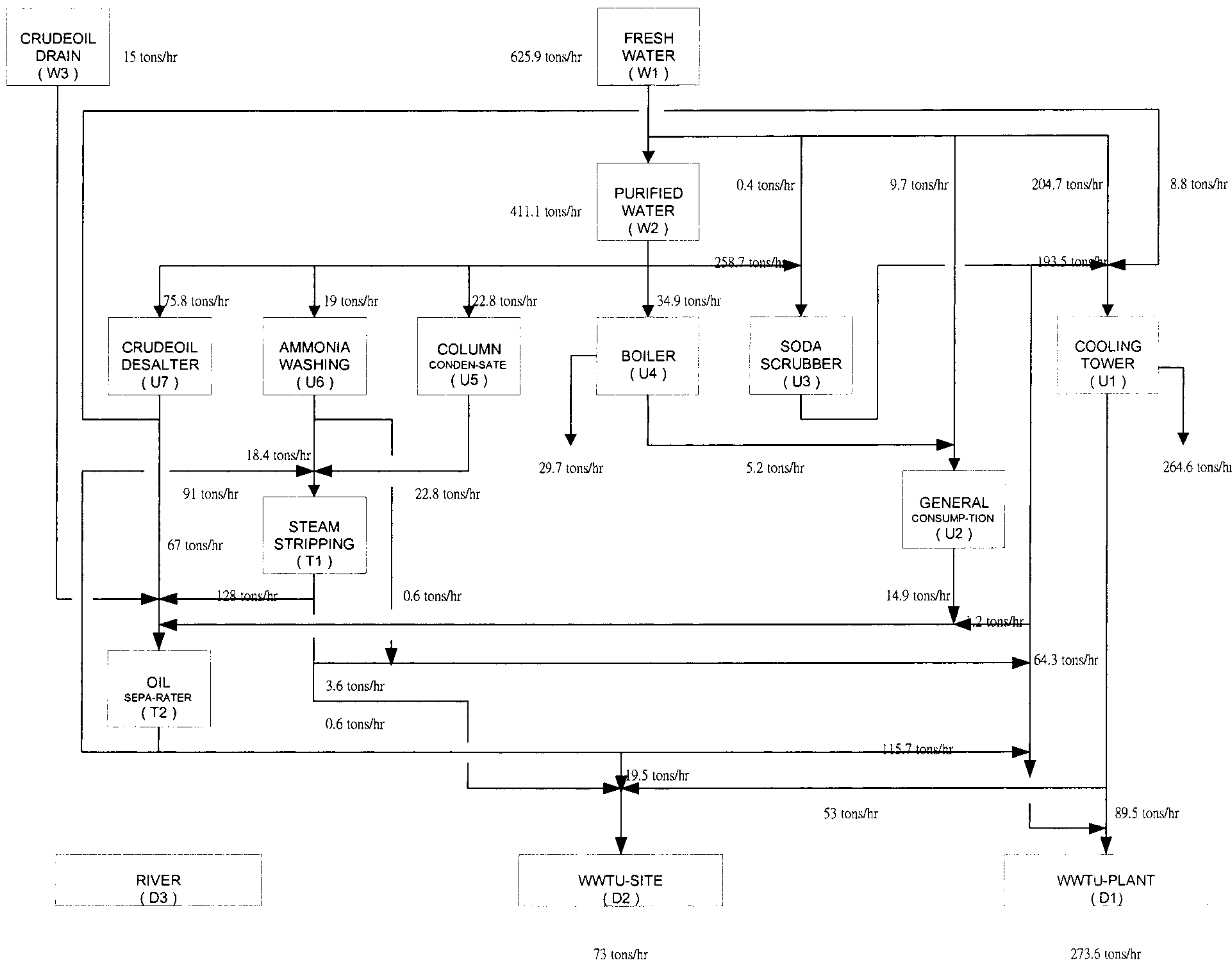

Figure 12. Block diagram of a least-consumption WUTN in the refinery. Case 2: The superstructure does not contain mixers and repeated units.

tions, it may be more appropriate to assume that outlet concentration of a solute k is constant since it is dependent only upon the operating conditions of the unit, i.e.

$$C_{ik}^{X} = \lambda_{ik}^{X} \quad i \in \mathbf{U} \quad k \in \mathbf{S} \tag{A5}$$

where λ_{ik}^{X} is a constant and also a design parameter. An example for 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.

$$B_{ik}^{X} \leq \beta_{ik}^{X} \quad i \in \mathbf{U} \quad k \in \mathbf{S} \tag{A6}$$

and

$$C_{ik}^{X} \leq \gamma_{ik}^{X} \quad i \in \mathbf{U} \quad k \in \mathbf{S} \tag{A7}$$

where β_{ik}^{X} and γ_{ik}^{X} denote respectively the maximum allowable concentrations of solute k at the inlet and outlet of unit i. Notice that the maximum allowable concentrations are also constant parameters which must be determined individually according to design considerations of each unit.

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.

$$Y_j = \bar{Y}_j + L_j \quad j \in \mathbf{T} \tag{A8}$$

and

$$Y_j B_{jk}^{Y} = M_{jk} + \bar{Y}_j C_{jk}^{Y} + L_j D_{jk}^{Y} \quad j \in \mathbf{T} \quad k \in \mathbf{S} \tag{A9}$$

where Y_j and $\bar{Y}_j$ 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 like stripping, absorption and solvent extraction; L_j denotes the corresponding water loss in operations such as evaporation, filtration, and membrane separation, etc.; B_{jk}^{Y} and C_{jk}^{Y} are used to represent, respectively, the inlet and outlet concentrations of solute k, and D_{jk}^{Y} is the concentration of solute k in the lost water.

In this work, the water loss is modeled with the following relation:

$$L_j = \phi_j Y_j \quad j \in \mathbf{T} \tag{A10}$$

where ϕ_j is a design parameter that must be estimated beforehand. It is assumed in this work that $\phi_j = 0$, when M_{jk} is positive in a typical mass exchanger or a biological or chemical treatment process. In other water-treatment units, the water quality of product stream is improved mainly by producing an additional more concentrated output stream, e.g., membrane separation, evaporation,

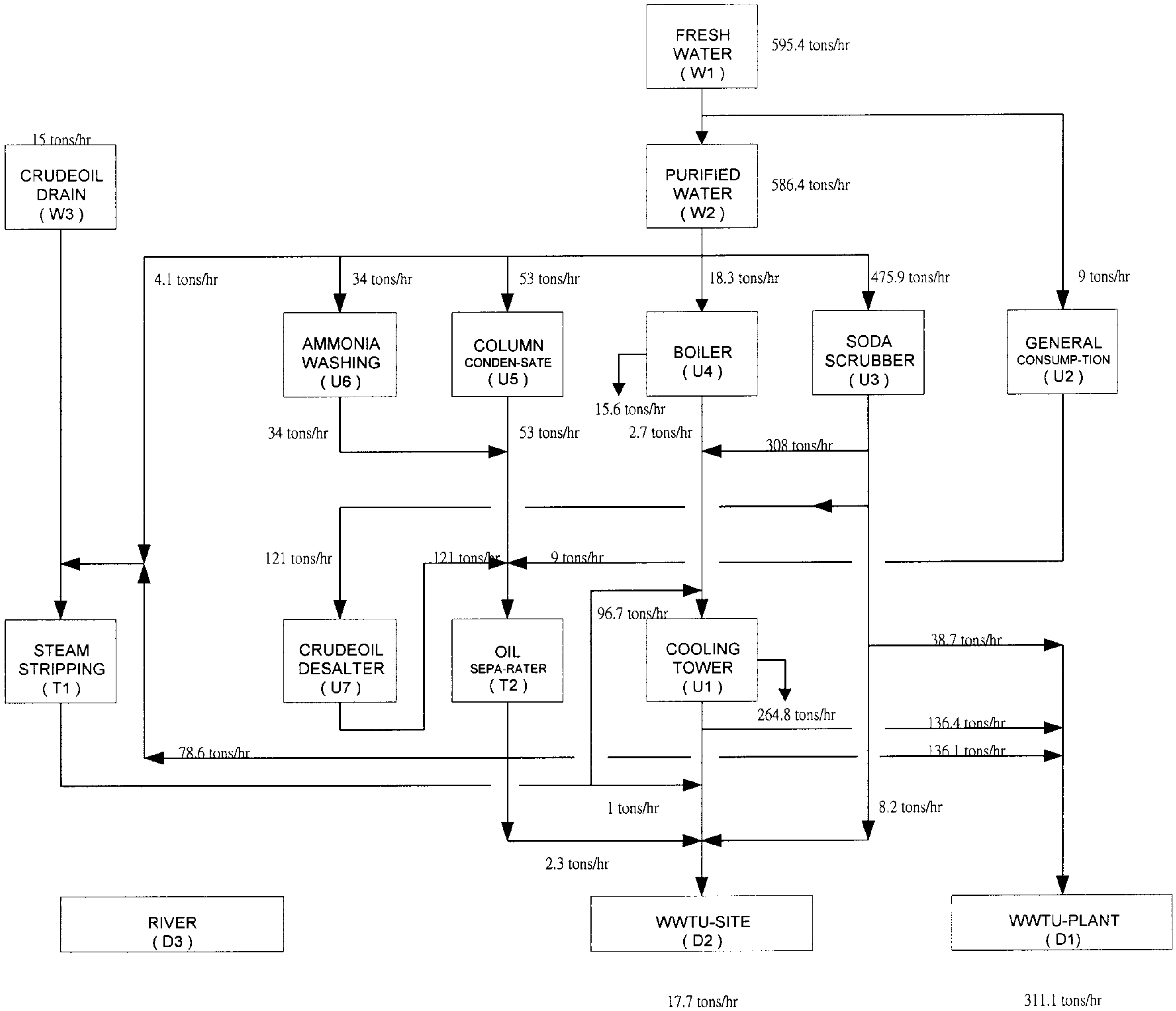

Figure 13. Block diagram of a least-consumption WUTN in the refinery. Case 3: There are three mixers in the superstructure.

and filtration, etc. In these cases, the term M_{jk} must be set to zero. Since the mass load cannot be predetermined in the former case and D^Y_{jk} is usually *not* negligible in the latter, additional equality constraints must be introduced to avoid unreasonable solutions. Two alternatives have been adopted. The first one is concerned with the removal ratio ψ_{jk}, i.e.

$$\frac{Y_j B^Y_{jk} - \bar{Y}_j C^Y_{jk}}{Y_j B^Y_{jk}} = \psi_{jk} \quad j \in \mathbf{T} \quad k \in \mathbf{S} \qquad \text{(A11)}$$

where ψ_{jk} denotes the efficiency of removing solute k in unit j and it is also considered a constant design parameter. Conceivably, a large number of treatment processes, e.g. filtration, centrifugal separation, biological treatment, etc., can be approximately modeled using this approach. On the other hand, if a process is believed to be equilibrium controlled, it may be better described with the following formulation:

$$C^Y_{jk} = \lambda^Y_{jk} \quad j \in \mathbf{T} \quad k \in \mathbf{S} \qquad \text{(A12)}$$

where λ^Y_{jk} denotes the constant concentration of solute k achieved at the exit of unit j. Examples of this type of operations include stripping, extraction, and 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.

$$B^Y_{jk} \le \beta^Y_{jk} \quad j \in \mathbf{T} \quad k \in \mathbf{S} \qquad \text{(A13)}$$

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

$$Y_j \le \eta_j \quad j \in \mathbf{T} \qquad \text{(A14)}$$

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

The Mixers. The mixers are used in superstructure mainly to introduce more options in WUTN design. A mixer is in fact a fictitious unit installed between a mixing node and a splitting node. The inlet and outlet conditions of this unit are identical, i.e.

$$R_n = \bar{R}_n \quad n \in \mathbf{X} \qquad \text{(A15)}$$

$$B^R_{nk} = C^R_{nk} \quad n \in \mathbf{X} \quad k \in \mathbf{C} \qquad \text{(A16)}$$

where R_n and $\bar{R}_n$ represent respectively the water flow rates at the inlet and outlet of unit n; B_{nk}^R and C_{nk}^R denote respectively the concentrations of solute k in the input and output streams of unit n.

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