PROCESS DESIGN AND CONTROL

A Mathematical Programming Model for Water Usage and Treatment Network Design

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A mathematical programming model is proposed in this paper for determining the optimal water usage and treatment network (WUTN) in any chemical plant, which features the least amount of fresh water consumption and/or minimum wastewater treatment capacity. In particular, because design equations of all wastewater treatment facilities and all units which utilize either process or utility water are included in the model, more comprehensive integration on a plant-wide scale can be achieved. In comparison with the available technologies, the proposed method is more reliable, more accurate, and much faster in synthesizing the WUTNs. Furthermore, more cost-efficient alternatives may be identified in certain design cases.

Introduction

Process integration, especially energy integration, has always been an active research area in process system engineering since the late 1970s. In fact, the design techniques for heat recovery systems have already matured. For example, Pinch analysis of heat exchanger networks (HENs) has been proven effective in many practical applications.[1] On the other hand, because of its obvious implications in pollution prevention, mass integration also became a subject of growing importance in recent years. The design method for mass exchanger networks (MENs) was shown to be a natural extension of that used for HENs.[2] Thus, the potential benefits of process integration are multifaceted, e.g., energy saving, waste minimization, cost reduction, etc.

A sufficient water supply is essential for running any commercial chemical process. This is because water may be used in almost every aspect 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, make-up 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, its demand has been increased dramatically in modern age because of 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.[3] first proposed a nonlinear programming formulation to solve the water allocation problem in a refinery. In the works of Wang and Smith[4,5] and Kuo and Smith,[6,7] 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. There are, however, shortcomings in this approach which require further attention:

(1) Although the minimum water consumption rate can be calculated with Pinch analysis for simple idealized systems,[8] it is difficult to identify the minimum fresh-water rate or wastewater treatment capacity for more realistic systems, especially the ones with multiple sources and sinks and those containing both water-using and water-treatment operations that result in water losses.

(2) Because the composite curve and network structure must be constructed manually, it is quite tedious, if not overwhelming, to implement this method for multisolute systems. Furthermore, the quality of the final design depends largely on the user's experience and thus may not be consistent.

(3) Although the interactions between the water-using, regeneration, and effluent treatment networks can be handled with an iterative procedure, these subsystems were still constructed individually. As a result, opportunities of integrating different types of

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10.1021/ie990043s CCC: $18.00
Published on Web 06/10/1999

water consumption/treatment units within a unified framework may be overlooked.

Another possible alternative is to formulate the water usage and treatment network (WUTN) design problem with the mass integration framework proposed by El-Halwagi et al.[9] Although this approach is considered more general, there are needs to address the problem from a different perspective. In particular, although a waste interception network (WIN) in this framework can be designed to reduce a target pollutant to a specified level, the resulting process configuration does not ensure optimal water utilization and distribution. Further, the mathematical formulation for WINs may not be suitable for our purpose for the following reasons:

(1) The quality of water is, in fact, characterized by more than one index.[10] Some of them may not even be affected by the target pollutant, e.g., PH, hardness, and turbidity. Thus, it is misleading to design a WUTN by adopting a "species viewpoint" on the basis of one pollutant.

(2) Wastewater streams coming out of various water-using units are viewed as the sources of rich streams containing the target pollutant in a WIN. However, as mentioned before, fresh and/or used water may also be the MSAs for other species in another WIN of the same plant. Thus, it is desirable to integrate multiple WINs so that potentially better WUTN configurations can be generated.

(3) Not all water-treatment processes can be described with the available models for mass exchangers or waste interceptors. For examples, biological treatment, flotation, filtration, and centrifugal separation cannot be treated as equilibrium-stage operations or differential contactors.

(4) Not all water-using units can be modeled as sinks/generators in the mass integration framework, e.g., the reactors using water as the reactant, the boilers and cooling towers that consume make-up waters, etc.

To overcome the above problems, a mathematical programming model is developed in this work to finalize the optimal WUTN design. Conceivably, this model can be used after completing the preliminary grass-roots flowsheet obtained with any of the available methods or simply for revamping an existing process. Various objective functions can be adopted in the model, e.g., the fresh water consumption rate, wastewater treatment capacity, operating cost, etc. This approach is considered to be reliable, versatile, and more comprehensive. Several simple examples are presented in this paper to support our viewpoint. Also, it should be noted that the effects of incorporating *repeated* water-treatment units in WUTN can be easily studied with the proposed mathematical program. The benefits of such a design practice are clearly demonstrated in one of the examples. Finally, we have successfully applied this model to two industrial problems. The case study involving the retrofit design of WUTN in a refinery is reported in detail at the end of this paper.

The Unit Models

Although there are three often-discussed elements in WUTN, i.e., the effluent treatment subsystem, the water use/reuse subsystem, and the regeneration subsystem, the equipment considered in the present study is only divided into two categories, i.e., water-using units and water-treatment units. This is due to the fact that units in the effluent treatment subsystem and also in the water regeneration subsystem are installed essentially for the same purpose, i.e., improving water quality. Thus, the same types of equipment can often be used in both cases. A description of the unit models adopted in our work is presented in the sequel:

Water-Using Units. As mentioned before, the plant operations that consume water or steam can be treated as sinks/generators in the mass integration framework suggested by El-Halwagi et al.[9] For illustration convenience, they are further classified into three types here:

1. Reaction: Water/steam may be either a reactant in hydrolysis reactions or, in many aqueous-phase reactions, simply an inert solvent.

2. Separation: Water or steam is used mainly as a MSA in separation processes such as absorption, extraction, leaching, stripping, etc.

3. Utility Generation: Both hot and cold utility generation equipment are considered here, i.e., the steam boiler and cooling tower. Let us consider these two cases separately.

(1) The utility steams may be utilized for driving turbines and heating process streams in a chemical plant. Although the resulting condensates are, in general, recovered and reused, a significant portion could still be lost in the process. In addition, notice that blow-down is a routine and necessary practice to prevent fouling and corrosion in the boiler. As a result, a steady supply of make-up water should always be maintained in operating the steam boiler.

(2) The cooling tower is also an essential equipment for plant operation. Its water throughput is often the highest one among all water-using units in the plant. Although the cooling water is always recycled after use, vaporization in the tower is inevitable. Because the concentration of nonvolatile solutes may build up, periodical water blow-down and make-up are also necessary for operating the cooling tower.

After an overview of various water-using units is presented, let us now introduce the definitions of a unit set and a species set to facilitate development of a concise formulation for the optimization problem, i.e.

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

$$\mathbf{S} = \{k|k \text{ is the label of a solute in aqueous phase which affects water quality}\} \quad (2)$$

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

$$X_i = \bar{X}_i + \nu_i \qquad i \in \mathbf{U} \quad (3)$$

where X_i and $\bar{X}_i$ denote the water flow rates at respectively 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 consumed. In the case of nonzero water loss, ν_i becomes a design parameter which must be determined according to the operating conditions of the unit before solving the mathematical program. Notice that, in order 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.

$$X_i B_{ik}^X + \mu_{ik} = \bar{X}_i C_{ik}^X + \nu_i D_{ik}^X \qquad i \in \mathbf{U} \quad k \in \mathbf{S} \qquad (4)$$

where B_{ik}^X and C_{ik}^X represent the concentrations of solute k at respectively 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 the reaction, μ_{ik} can be negative, zero, or positive depending on whether solute k is a reactant, an inert, 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 the 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 3 and 4 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.

$$D_{ik}^X = 0 \qquad i \in \mathbf{U} \quad k \in \mathbf{S} \qquad (5)$$

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 upon the operating conditions of the unit, i.e.

$$C_{ik}^X = \lambda_{ik}^X \qquad i \in \mathbf{U} \quad k \in \mathbf{S} \qquad (6)$$

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.

$$B_{ik}^X \le \beta_{ik}^X \qquad i \in \mathbf{U} \quad k \in \mathbf{S} \qquad (7)$$

and

$$C_{ik}^X \le \gamma_{ik}^X \qquad i \in \mathbf{U} \quad k \in \mathbf{S} \qquad (8)$$

where β_{ik}^X and γ_{ik}^X denote the maximum allowable concentrations of solute k at respectively 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. In most process plants, wastewater treatment is accomplished by collecting all aqueous effluents in a common sewer and then treating them in a central facility before releasing them into the environment. This centralized treatment process may include all or part of the so-called primary, secondary, and tertiary stages. However, recent studies reveal that a segregated treatment strategy, i.e., processing different effluents individually in the first instance and combining them only when it is necessary, could have significant advantages over the traditional approach.[5,6] Although the implementation philosophy has been changed, the water-treatment units adopted in the segregated scheme remain the same. Because a detailed survey of water reclamation technologies can be found in the literature, e.g., Zinkus et al.,[10] a review of treatment units is omitted here for the sake of conciseness.

A similar formulation has been adopted to model the water-treatment processes. Let us now introduce the definition of another unit set, i.e.

$$\mathbf{T} = \{j | j \text{ is the label of a water-treatment unit in the plant; } j = 1, 2, ..., N_t\} \qquad (9)$$

As mentioned before, not all effluent processing units can be considered as the conventional mass exchangers or waste interceptors. Thus, 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.

$$Y_j = \bar{Y}_j + L_j \qquad j \in \mathbf{T} \qquad (10)$$

and

$$Y_j B_{jk}^Y = M_{jk} + \bar{Y}_j C_{jk}^Y + L_j D_{jk}^Y \qquad j \in \mathbf{T} \quad k \in \mathbf{S} \qquad (11)$$

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:

$$L_j = \phi_j Y_j \qquad j \in \mathbf{T} \qquad (12)$$

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 the product stream is improved mainly by producing an additional more concentrated output stream, e.g., membrane separation, evaporation, filtration, etc. In these cases, the term M_{jk} must be set to zero. Because the mass load cannot be predetermined in the former case and D_{jk}^Y 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.

$$\frac{Y_j B_{jk}^Y - \bar{Y}_j C_{jk}^Y}{Y_j B_{jk}^Y} = \psi_{jk} \qquad j \in \mathbf{T} \quad k \in \mathbf{S} \qquad (13)$$

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:

$$C_{jk}^{Y} = \lambda_{jk}^{Y} \qquad j \in \mathbf{T} \quad k \in \mathbf{S} \tag{14}$$

where λ_{jk}^{X} 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 7, i.e.

$$B_{jk}^{Y} \le \beta_{jk}^{Y} \qquad j \in \mathbf{T} \quad k \in \mathbf{S} \tag{15}$$

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

$$Y_j \le \eta_j \qquad j \in \mathbf{T} \tag{16}$$

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

Water Sources and Sinks

As mentioned before, our design objective is to optimize water distribution within a process plant. Consequently, the scope of this study is defined by the plant boundary. This is considered as a comprehensive but practical approach because the decisions concerning flowsheet modifications are most likely to be made by plant-level managers. The external water sources considered in this work can be categorized into two types:

(1) Primary Water: The most dependable sources of industrial water are those available in the environment. They can be further classified as surface and underground waters. Examples of the former include waters from rivers, lakes, reservoirs, seas, etc. 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. Notice that, because the requirements of these units are not the same, waters of different qualities must be produced accordingly with various treatment methods, e.g., a simple softening process can be used to create the liquid MSAs for mass exchangers, an ionization process to treat boiler waters, and further evaporation to generate steams for stripping and purging. 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. For example, secondary waters may be generated by reaction in the TPA (terephthalic acid) process and, in a refinery, by settling and draining the crude oil for a purification purpose. 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, a review of all potential water sinks is also presented below:

(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, 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. Further, in revamping applications, it may be necessary to treat the existing central treatment process in the plant as a sink also.

(3) Type C: As mentioned before, 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 in our studies. One is used to collect all loss streams from the former units and the other is for the latter.

For the purpose of achieving consistency in notation, five additional sets are defined on the basis of the above classification:

$$\mathbf{I}_1 = \{p | p \text{ is the label of a primary source for WUTN; } p = 1, 2, ..., N_p\} \tag{17}$$

$$\mathbf{I}_2 = \{s | s \text{ is the label of a secondary source for WUTN; } s = 1, 2, ..., N_s\} \tag{18}$$

$$\mathbf{O}_A = \{a | a \text{ is the label of a type A sink for WUTN; } a = 1, 2, ..., N_a\} \tag{19}$$

$$\mathbf{O}_B = \{b | b \text{ is the label of a type B sink for WUTN; } b = 1, 2, .., N_b\} \tag{20}$$

$$\mathbf{O}_C = \{c | c \text{ is the label of a type C sink for WUTN; } c = U \text{ or } T\} \tag{21}$$

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 Takama et al.[3] It contains additional features, e.g., water losses, multiple sources, and sinks, to address practical concerns in realistic applications. A simple construction procedure of this general structure is presented below:

1. Place a mixer node at the inlet of every water-using and water-treatment unit. The merged stream is sent to the unit.

2. Place a mixer node before each type A sink. The merged stream is discharged to the sink.

3. Place a mixer node before each type B sink. The merged stream is discharged to the sink.

4. Place two mixer 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.

5. Place a splitter node after each primary source. The split branches of every such node are connected to all of the mixer nodes established in step 1.

6. Place a splitter node after each secondary source. The split branches of every such node are connected to all of the mixer nodes established in steps 1−3.

7. Place a splitter node at the exit of every water-using and water-treatment unit. The split branches of

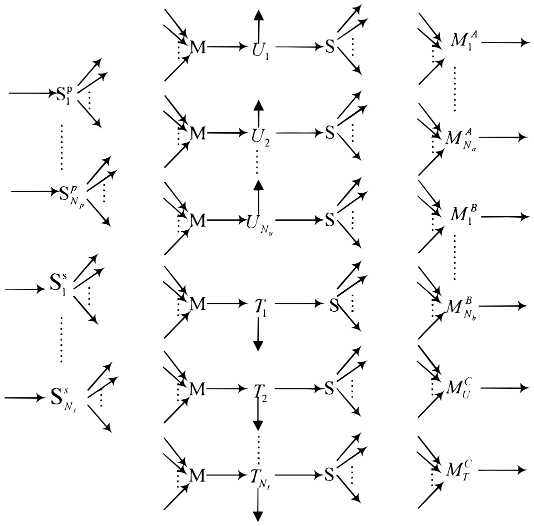

Figure 1. General superstructure for water usage and treatment networks.

every such node are connected to all of the mixer nodes installed in steps 1−3 *except* the one before the same unit.

This scheme is 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 splitter 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 the mixer nodes before sinks of respectively types A and B; M_U^C and M_T^C denote the mixers 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 mixer and splitter attached before and after this unit; and, similarly, $M - T_t - S$ ($t \in \mathbf{T}$) represents the tth water-treatment unit and the attached mixer and splitter. 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. The unit and node models should all be included as the constraints of this optimization problem. The unit models adopted in this work have already been discussed previously. On the other hand, the descriptions of node models are omitted in this paper for the sake of brevity. Notice that equality constraints used in these node models are simply water and solute balances. In addition, inequality constraints concerning wastewater flow rate and/or pollutant concentrations after the mixers M_a^A's and M_b^B's must also be imposed to satisfy environmental requirements at type A and B sinks. Finally, it is assumed that the solute concentrations in each primary and secondary source are given and the supply of any secondary water is limited.

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

$$F^C = \sum_{u \in \mathbf{U}} \omega_u^X X_u + \sum_{t \in \mathbf{T}} \omega_t^Y Y_t + \sum_{b \in \mathbf{O}_B} \omega_b^Z Z_b^B \tag{22}$$

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 respectively the uth water-using unit, the tth water-treatment unit, and the bth sink of type B.

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

$$F^W = \sum_{p \in \mathbf{I}_1} W_p^P \tag{23}$$

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

$$F^W = \sum_{a \in \mathbf{O}_A} Z_a^A + \sum_{b \in \mathbf{O}_B} Z_b^B + (Z_U^C + Z_T^C) \tag{24}$$

where Z_a^A denotes the discharge rate to the ath sink of type A and 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 23 or eq 24. Thus, the latter will not be considered in the following examples.

Simple Examples

Several fictitious examples are presented here to illustrate the implementation procedure and to demonstrate the advantages of our approach. The benefits of using a mathematical programming model are manifold. It is obviously reliable because of the fact that, in solving large-size multisolute WUTN design problems, human errors can be avoided. It is versatile because the proposed mathematical program can be easily adapted for a wide range of revamp and grass-roots design applications. It is also comprehensive because more alternatives and, in certain cases, more appropriate designs can be identified when compared with the manual approach. Some of them may even be neglected by experienced engineers.

As in other nonlinear optimization problems, the initialization issues must be addressed. In general, any feasible solution can be adopted as the initial starting point. To generate such a solution, one can make use of the Pinch method or simply solve the equality constraints of the NLP model by fixing the extra degree of freedom with "reasonable" guesses of the key design variables. In practical applications, these guesses are not difficult to obtain because the stream data of a base-case flowsheet are often available.

Example 1. Although our mathematical program was written for the entire WUTN, it can be applied locally to design a water usage network by removing all of the water-treatment units from the superstructure. Let us consider a design problem considered by Wang and

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

unit no. i	mass load μ_i (kg/h)	max inlet conc β_i (ppm)	max outlet conc γ_i (ppm)
1	2	0	100
2	5	50	100
3	30	50	800
4	4	400	800

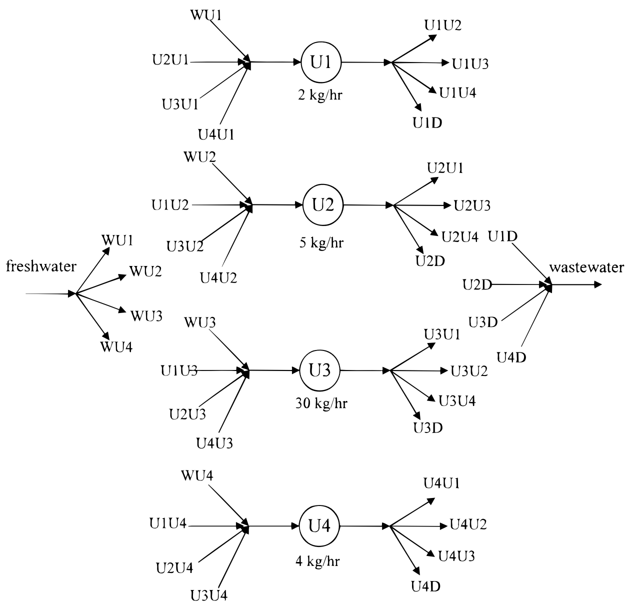

Figure 2. Superstructure for example 1.

Smith.[4] In this problem, only one fresh-water source is available for use. The process data of water-using units are repeated in Table 1. Notice that, because there is only one solute, the second subscripts of the symbols μ_{ik}, β_{ik}^{X}, and γ_{ik}^{X} are dropped in this table. In addition, the superscripts of the last two are omitted because all water-treatment units are excluded in this example.

The first step in solving this problem is to build a superstructure (see Figure 2). Note that there is only one sink because wastewater treatment is not the concern of this design and there is no water loss in any of the units. After the unit and node models are constructed, the resulting mathematical program can be solved with a commercial software, e.g., GAMS,[11] on a Pentium PC using the fresh-water flow rate, i.e., eq 23, as the objective function. To facilitate understanding, the GAMS input file used in this case is provided as Supporting Information. The minimum water consumption rate in this case was found to be 90 tons/h. One of the optimal WUTN designs is presented in Figure 3a. Notice this result is actually the same as that obtained with the available method.

On the other hand, it should be noted that more than one equally acceptable alternative can be easily generated by introducing perturbations to the initial guesses and solving the problem repeatedly. Two such alternative networks are presented in Figure 3b,c. Thus, it is clear that, if the proposed approach is adopted, several network configurations can be quickly made available to the designer this way. A final decision can then be reached on the basis of practical considerations not included in the mathematical formulations. As a result, the iteration process usually needed in creating a design can be greatly shortened or eliminated completely. □

Example 2. Let us next consider an effluent treatment network design problem studied by Wang and Smith.[5] The wastewater stream data and the treatment process data for this problem are presented in Tables 2 and 3, respectively. Notice again that the second subscripts of the symbols ψ_{ik} and β_{ik}^{Y} are dropped in Table 3 because there is only one solute. Also, the superscript of the latter is omitted because only water-treatment units are involved. In this problem, the concentration of wastewater is required to be reduced to 10 ppm before discharging into the environment.

On the basis of the superstructure given in Figure 4, a mathematical program can be constructed. The objec-

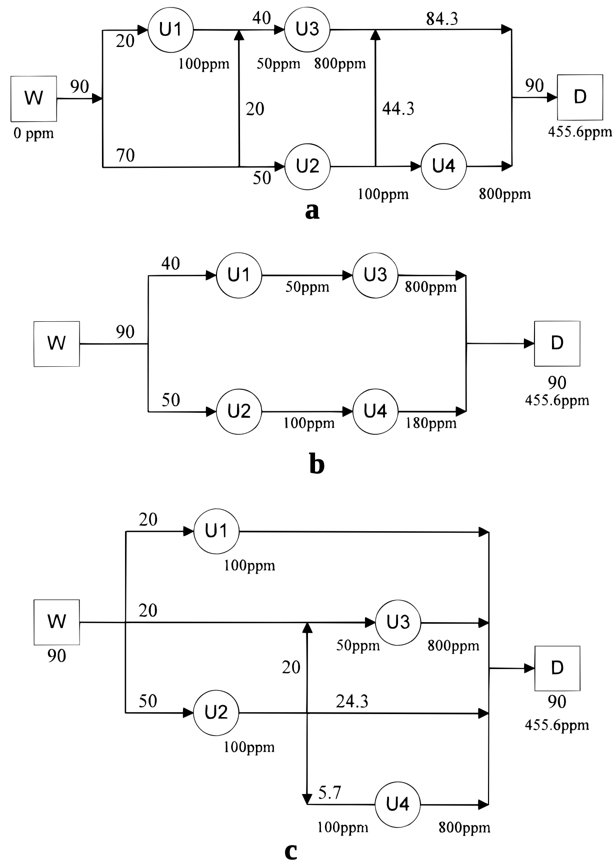

Figure 3. (a) Candidate WUTN structure for example 1, option 1. (b) Candidate WUTN structure for example 1, option 2. (c) Candidate WUTN structure for example 1, option 3.

Table 2. Wastewater Stream Data in Example 2

stream no.	flow rate (tons/h)	conc (ppm)
1	60	400
2	20	800

Table 3. Process Data of Water-Treatment Units in Example 2

unit no. j	removal ratio ψ_j	max inlet conc β_j (ppm)
1	0.99	200
2	0.80	1000

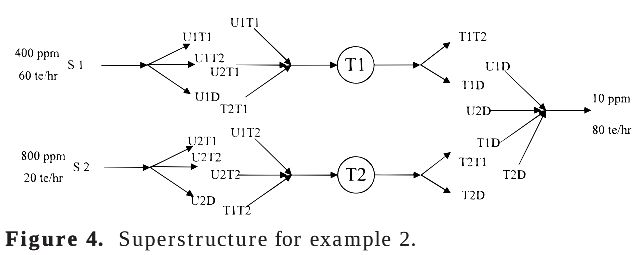

Figure 4. Superstructure for example 2.

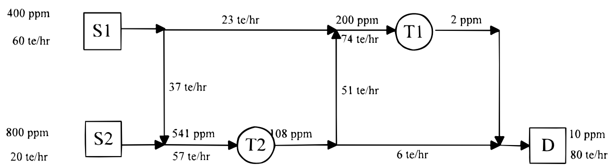

Figure 5. Candidate WUTN structure for example 2.

Table 4. Water Sources of Example 3

	conc (ppm)		
source no.	solute A	solute B	max flow rate (tons/h)
1	0.1	0.1	∞
2	60	28	30
3	1800	1200	40

Table 5. Process Data of Water-Using Units in Example 3

unit no. i	solute k	mass load μ_{ik} (kg/h)	max inlet conc β^{X}_{ik} (ppm)	max outlet conc γ^{X}_{ik} (ppm)	water loss ν_i (tons/h)
1	A	8.0	0.1	100.1	0
	B	4.0	25.0	75.0	
2	A	11.2	80.0	240.0	0
	B	4.2	30.0	90.0	
3	A	0.0	8.0	8.0	15.0
	B	0.0	5.0	5.0	

Table 6. Process Data of Water-Treatment Units in Example 3

unit no. j	solute k	removal ratio ψ_{jk}	outlet conc λ^{Y}_{jk} (ppm)	max inlet conc β^{Y}_{jk} (ppm)	max through-put η_j (tons/h)
1	A	0.90			125
	B	0.80			
2	A	0.20			125
	B	0.95			
3	A		5	200	125
	B		5	100	

tive function for this case is the total capacity of the two treatment units, i.e., $F^{C} = Y_1 + Y_2$ and $\omega^{Y}_1 = \omega^{Y}_2 = 1$. It was found in one of the optimal solutions that the flow rates through T_1 and T_2 are 74 and 57 tons/h, respectively. The corresponding network configuration is presented in Figure 5. When compared with the original result, i.e., 153 tons/h, this solution is about 17% lower. Note that it may be possible to achieve the same reduction with a modified version of the Pinch method.[6] However, a considerable effort in developing the improved design from an initial solution is still needed with such an evolutionary strategy. □

Example 3. Consider a fictitious process with three 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 4. Notice that primary water is available only from the first source. Also, because of government regulations, the concentrations of both solutes in the wastewater must be lowered to at least 10 ppm before discharging to the environment. The process data of existing water-using units can be found in Table 5. Notice that only operation U_3 causes a loss of 15 tons/h, and it is assumed that eq 5 is applicable in this case, i.e., $D^{X}_{3A} = D^{X}_{3B} = 0$. The process data of the available water-treatment units are given in Table 6 in which the first two are characterized with constant removal ratios and the third is characterized with a constant outlet concentration. Further, none of these operations result in water loss, i.e., $\phi_1 = \phi_2 = \phi_3 = 0$.

The same procedure was followed to synthesize the optimal WUTNs according to the objective functions defined in eqs 22 and 23. In the former case, the

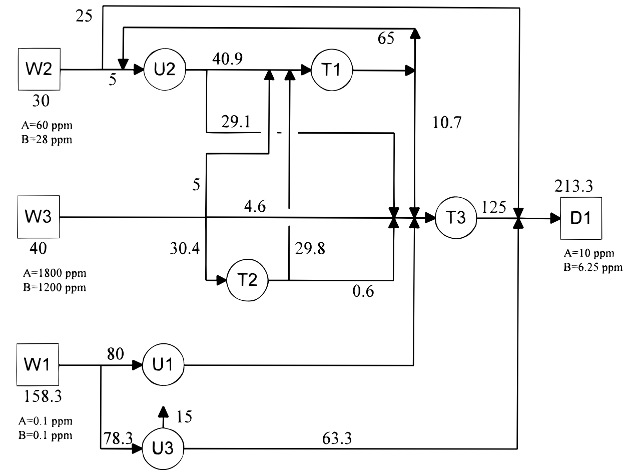

Figure 6. WUTN structure of a cost-optimal design for example 3, case 1: one T_1, one T_2, and one T_3.

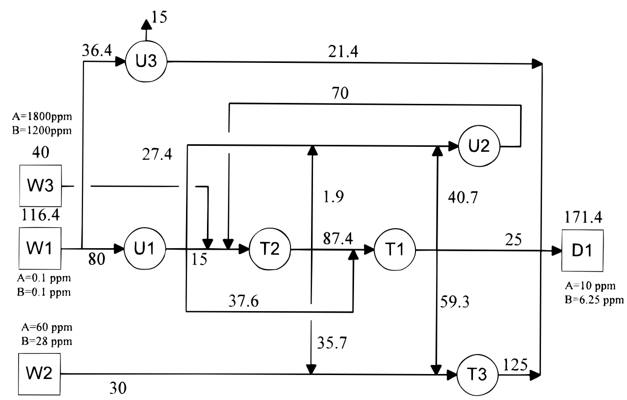

Figure 7. WUTN structure of a least-consumption design for example 3, case 1: one T_1, one T_2, and one T_3.

Table 7. Operating Conditions of Process Units in the Cost-Optimal WUTN for Example 3, Case 1: One T_1, One T_2, and One T_3

process unit	throughput (tons/h)	solute	inlet conc (ppm)	outlet conc (ppm)
U_1	80	A	0.1	100.1
		B	0.1	50.1
U_2	70	A	80	240
		B	30	90
U_3	78.3	A	0.1	0.124
		B	0.1	0.124
T_1	75.7	A	815.4	81.5
		B	150.8	30.2
T_2	30.5	A	1800	1440
		B	1200	60
T_3	125	A	200	5
		B	100	5

minimum-cost WUTN was obtained by assuming equal weighting factors in F^{C}; i.e., let $\omega^{X}_1 = \omega^{X}_2 = \omega^{X}_3 = \omega^{Y}_1 = \omega^{Y}_2 = \omega^{Y}_3 = 1$. The corresponding 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 7. On the other hand, if water conservation (or waste minimization) is our design objective, an alternative WUTN configuration can be identified according to F^{W} (Figure 7). The detailed process data of each unit in this network are presented in Table 8. 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 fresh water (see Figure 6) will be higher than that

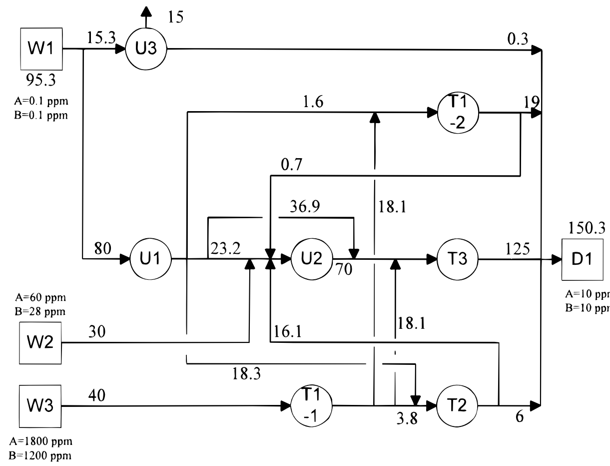

Figure 8. WUTN structure of a cost-optimal design for example 3, case 2: two T_1's, one T_2, and one T_3.

Table 8. Operating Conditions of Process Units in the Least-Consumption WUTN for Example 3, Case 1: One T_1, One T_2, and One T_3

process unit	throughput (tons/h)	solute	inlet conc (ppm)	outlet conc (ppm)
U_1	80	A	0.1	100.1
		B	0.1	50.1
U_2	30.5	A	80	240
		B	23.7	83.7
U_3	125	A	0.1	0.17
		B	0.1	0.17
T_1	125	A	434.4	43.4
		B	30.3	6.1
T_2	125	A	722.4	577.9
		B	436.9	21.8
T_3	125	A	200	5
		B	15.8	5

needed in the design obtained with objective function F^W (see Figure 7). However, a larger-than-minimum total capacity will always be required if one tries to reduce the use of fresh water in the minimum-cost WUTN. This point is supported by the fact that, in Table 8, the throughputs in T_1, T_2, and T_3 reach their respective upper bounds given in Table 5.

Notice that the process conditions of the water-using units given in Table 5 are, in general, determined by the needs of the chemical process. In other words, these units exist as a part of the process itself. On the other hand, the water-treatment units listed in Table 6 can be viewed as equipment available for use. As long as the environmental requirements can be satisfied, the network configuration for wastewater treatment and, further, the *number* of each unit used in the network should not be limited. Consequently, it is necessary to access the effects of having *repeated* water-treatment units in WUTN.

Let us first consider the case when one more T_1 is introduced in the superstructure. The resulting cost-optimal WUTN is presented in Figure 8, and the corresponding process data are listed in Table 9. When compared with the data in Table 8, one can see that the total capacity is reduced from 459.5 to 372.1 tons/h. The results of minimizing F^W are provided in Figure 9 and Table 10, respectively. Again, significant savings in fresh water can be achieved, i.e., from 116.4 to 80 tons/h, by using two T_1's in WUTN.

Naturally, every other possible alternative can also be studied. These alternatives include all possible combinations of additional treatment units. Notice that

Table 9. Operating Conditions of Process Units in the Cost-Optimal WUTN for Example 3, Case 2: Two T_1's, One T_2, and One T_3

process unit	throughput (tons/h)	solute	inlet conc (ppm)	outlet conc (ppm)
U_1	80	A	0.1	100.1
		B	0.1	50.1
U_2	70	A	80	240
		B	30	90
U_3	15.3	A	0.1	5
		B	0.1	5
T_1-1	40	A	1800	180
		B	1200	240
T_1-2	19.7	A	173.4	17.3
		B	224.2	44.8
T_2	22.1	A	113.8	91
		B	82.7	4.1
T_3	125	A	190	5
		B	100	5

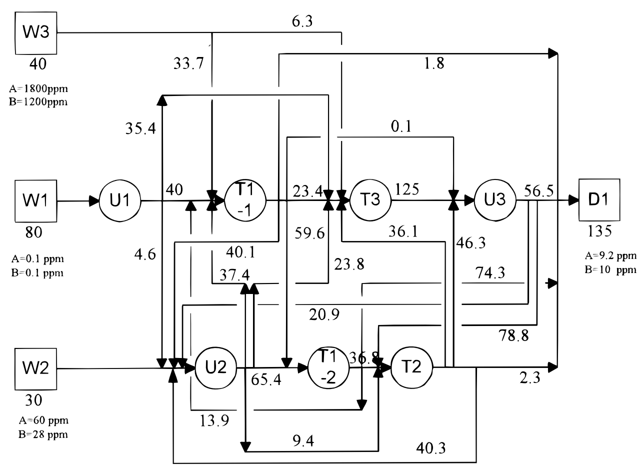

Figure 9. WUTN structure of a least-consumption design for example 3, case 2: two T_1's, one T_2, and one T_3.

Table 10. Operating Conditions of Process Units in the Least-Consumption WUTN for Example 3, Case 2: Two T_1's, One T_2, and One T_3

process unit	throughput (tons/h)	solute	inlet conc (ppm)	outlet conc (ppm)
U_1	80	A	0.1	100.1
		B	0.1	50.1
U_2	136	A	38.2	120.5
		B	29.9	60.8
U_3	171.4	A	7.3	8
		B	3.8	4.2
T_1-1	125	A	554.1	55.4
		B	359	71.8
T_1-2	125	A	89.5	8.9
		B	66	13.2
T_2	125	A	16.8	13.4
		B	11.1	0.6
T_3	125	A	156.5	5
		B	100	5

each of these design cases can be evaluated easily by adding one more unit to the mathematical program of a previously-solved case and using its solution as the initial guess. In these studies, it was concluded that no further cost reduction can be identified. However, the use of fresh water can be eliminated completely with three T_1's in the optimal WUTN (see Figure 10 and Table 11). □

Applications

Let us now apply the proposed methodology to a realistic problem concerning the retrofit of WUTN in a

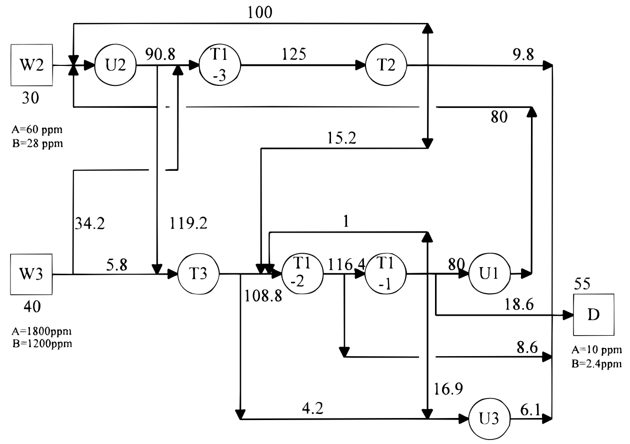

Figure 10. WUTN structure of a least-consumption design for example 3, case 3: three T_1's, one T_2, and one T_3.

Table 11. Operating Conditions of Process Units in the Least-Consumption WUTN for Example 3, Case 3: Three T_1's, One T_2, and One T_3

process unit	throughput (tons/h)	solute	inlet conc (ppm)	outlet conc (ppm)
U_1	80	A	0.1	100.1
		B	0.2	50.2
U_2	210	A	68.8	122.2
		B	24.8	44.8
U_3	21.1	A	1.1	3.9
		B	1.2	4.2
T_1-1	116.4	A	1	0.1
		B	1	0.2
T_1-2	125	A	10	1
		B	4.8	1
T_1-3	125	A	581.3	58.1
		B	360.9	72.2
T_2	125	A	58.1	46.5
		B	72.2	3.6
T_3	125	A	200	5
		B	98.4	5

refinery. A simplified block diagram of the original process can be found in Figure 11. The water consumed in this plant is taken primarily from a nearby reservoir. After various preliminary treatments, the primary waters can be made available basically at two quality levels. They are referred to as the *fresh water* and *purified water*, respectively, in this study. Because the crude oil often carries emulsified water, the purification operations, such as settling and draining, are indispensable in the topping plant. The wastewater collected from these operations can be viewed as a secondary source of WUTN. The process data of all of the water sources mentioned above are summarized in Table 12.

From Figure 11, one can see that the purified water is used for four different purposes:

(1) Desalination: Because inorganic salts, mostly chlorides, exist in the emulsified water, it is therefore necessary to apply purified water in the desalter to prepare crude oil for the distillation process downstream.

(2) Ammonia Wash: In the HDS treatment process of the heavy diesel and residuals, the desulfured fuels are separated by means of cooling/condensation. However, ammonium salts are also produced in solid form at the same time. Because they cause corrosion and blockage in the pipeline, washing becomes a routine operation in the refinery.

(3) Fractionation: Steam is injected in the fractionator to provide the needed energy for distillation. The

Table 12. Water Sources of the Refinery

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

steam is, of course, produced with a boiler in which only purified water can be used. For convenience, the vaporized water consumed in fractionation is treated as a primary water whose quality is the same as that utilized in desalination and ammonia wash.

(4) Steam Generation: The purified water should always be used for boiler make-up. The hot-utility generation system as a whole is regarded as a water-using unit in this work. Notice that part of the boiler-produced steam is used in fractionation and maybe other operations in the refinery. Thus, the inlet flow rate to this fictitious unit should be determined by subtracting the consumption rates of all such process steams from the actual make-up rate. Because the condensates of utility steams are recycled, the outputs of the unit should only include the blow-down and loss due to leakage.

In this refinery, the quality requirements of water used in several other operations are less stringent. Three of them are considered in this case study:

(1) Soda Scrubbing: In the final purification process of LPG, aqueous soda solution is used to extract sulfur impurities in the liquid product. Fresh water is used to prepare the solution for soda scrubbing.

(2) Cooling-Water Generation: Similar to the boiler, the entire cooling-water generation system is also viewed as a fictitious unit. Because all cooling waters are recycled and reused, the input of the unit should be the make-up water and the outputs should be blow-down water and evaporation loss in the cooling tower. The make-up water in this case does not have to be of the same quality as that of boiler make-up.

(3) General Consumption: Fresh water is also used for various miscellaneous purposes, e.g., equipment cleaning, fire fighting, purging, and other routine activities. Because their total consumption rate is significant when compared with those of other operations, *general consumption* is treated as a water-using operation in our mathematical program.

The process data of all water-using units considered in this case study are summarized in Table 13. Notice that no significant water loss occurs in any of these units except U_1 and U_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 5 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 6 is adopted in these situations, and the values of λ_{ik}^{X}'s are underlined in the table.

The refinery is located in a large industrial park with a centralized wastewater-treatment facility on site. The plant itself also has one for end-of-pipe treatment. The wastewaters must be treated to satisfy government requirements before they can be discharged into a river. Thus, three sinks can be considered in our mathematical program, and their process data are given in Table 14. The acronyms WWTU(PLANT) and WWTU(SITE) represent the centralized wastewater-treatment units in plant and on site, respectively.

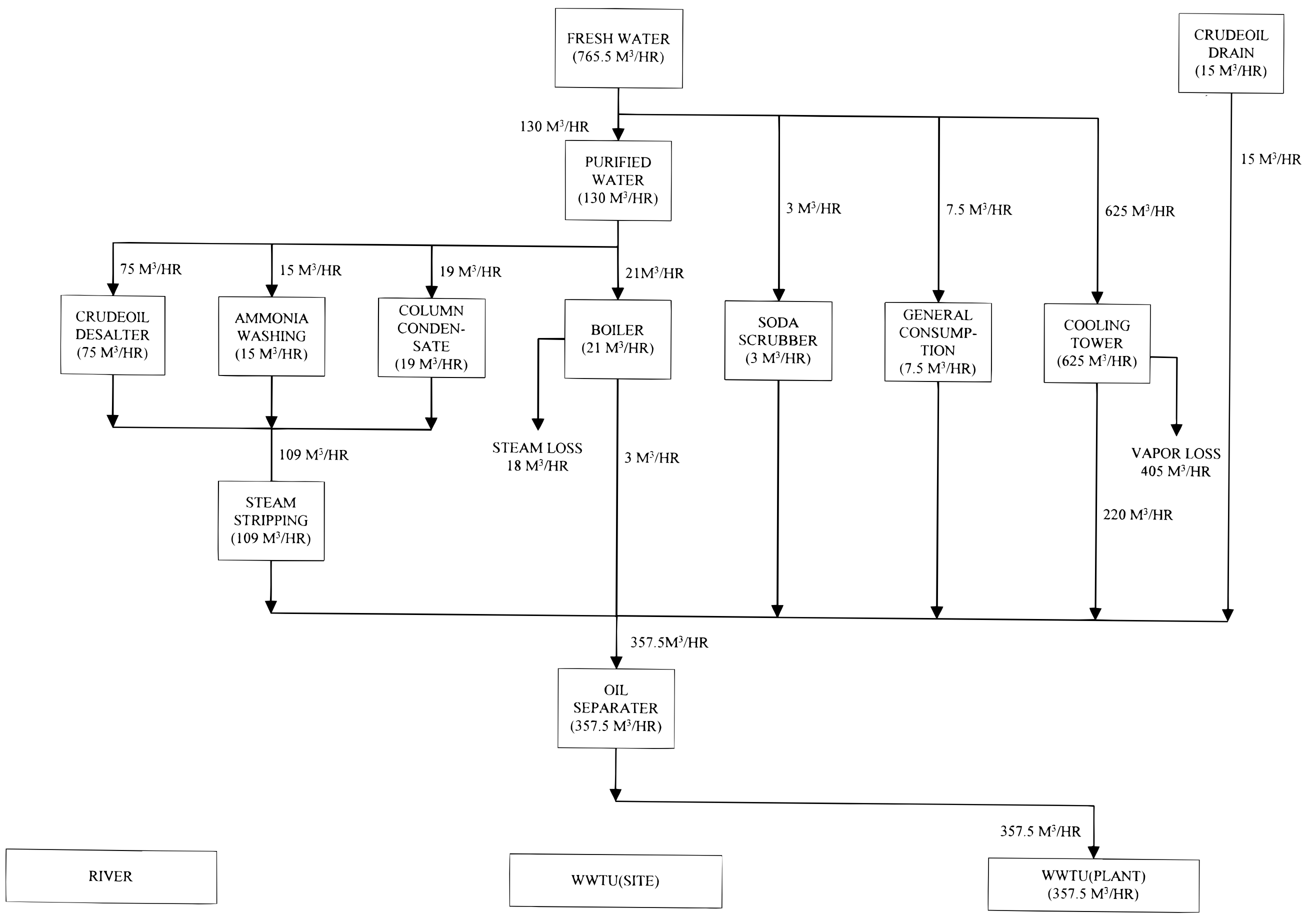

Figure 11. Block diagram of the original WUTN in the refinery.

Table 13. Process Data of Existing Water-Using Units in the Refinery

unit i	solute k	μ_{ik} (kg/h)	β_{ik}^{X} (ppm)	γ_{ik}^{X} (ppm)	ν_i (tons/h)
cooling tower (U_1)	salts	0	2500	3115	405
	organics	0	220	220	
	H_2S	0	45	45	
general consumption (U_2)	salts	7.125	300		0
	organics	52.5	50		
	H_2S	0.221	0		
soda scrubber (U_3)	salts	0.18	300	500	0
	organics	1.2	50	500	
	H_2S	1.75	5000	12500	
steam boiler (U_4)	salts	0	10	150	18
	organics	0	1	50	
	H_2S	0	0	0	
fractionation column (U_5)	salts	3.61	10	200	0
	organics	104.481	1	6500	
	H_2S	2.5	0	500	
ammonia wash (U_6)	salts	7.485	10	7500	0
	organics	81.75	50	6500	
	H_2S	3.2	50	480	
crude desalter (U_7)	salts	120.0	200	9500	0
	organics	480.0	100	6500	
	H_2S	1.875	20	45	

Table 14. Water Sinks of the Refinery

source	max conc (ppm)			max flow rate (tons/h)
	salts	organics	H_2S	
WWTU(PLANT)	364	759	24	360
WWTU(SITE)	300	600	20	200
river	50	200	10	∞

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

unit j	solute k	ψ_{jk}	η_j (tons/h)
steam stripper (T_1)	salts	0	150
	organics	0.25	
	H_2S	0.95	
API separator (T_2)	salts	0.25	400
	organics	0.55	
	H_2S	0	

Two additional water-treatment units are also present in the existing process. In general, high concentrations of H_2S, inorganic salts, and light hydrocarbons can be found in wastewaters generated from desalination, fractionation, and ammonia wash. Consequently, steam stripping is applied to remove H_2S and the light hydrocarbons from those streams. The resulting wastewater is combined with those from the boiler, cooling

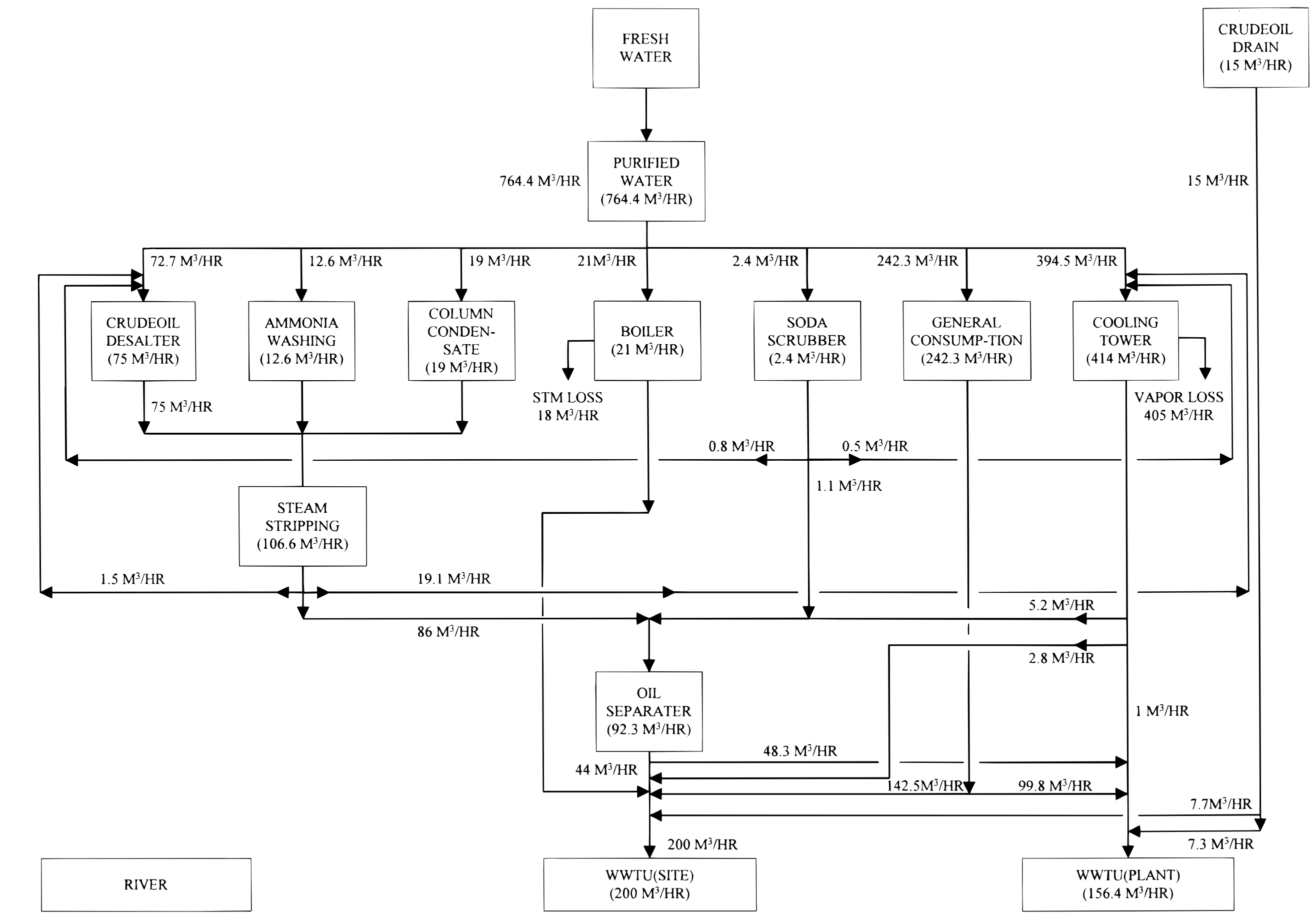

Figure 12. Block diagram of a cost-optimal WUTN in the refinery, case 1: API-treated water is not reused.

tower, soda scrubber, etc., in a common sewer. The output of sewer is then processed in a centralized facility. The process data of these two existing water-treatment units can be found in Table 15. Notice that eq 13 is 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.

In order to address other practical concerns in plant operation, additional constraints have been included in the formulation for WUTN synthesis.

(1) Because 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 splitter after T_2 and mixers before all water-using units.

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

(3) A minimum water-consumption level, i.e., 7.5 tons/h, is maintained for general use.

When those constraints are added, the mathematical program can be solved according to the objective function F^C or F^W. In the former case, because 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 should be 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 should be set to 1. The resulting cost-optimal design can be found in Figure 12. Notice that the fresh water used by this WUTN, i.e., 764.4 tons/h, is about the same as that required by the original design. Thus, the total discharge rates of both cases are also almost equal. On the other hand, the total throughput of the cost-optimal design is lower than that of the current practice. A 20% reduction in total throughput, i.e., from 1232 to 985.2 tons/h, can be achieved simply by rearranging the WUTN configuration. Under the cost structure implied in the objective function, it can be observed clearly from Figure 12 that the best revamping strategy for the present case is to upgrade the quality of water consumed in every water-using unit. Notice that all units now receive purified water although U_1 and U_7 also make use of some used and regenerated waters. As a result, the used waters from these units are much cleaner and thus can be sent directly to the sinks without treatment. Of course, the design strategy may not be the same if a different objective function is chosen to reflect the cost structure. Finally, notice that discharging into a river is not recommended in this case because the units T_1 and T_2 are not capable of treating wastewaters to meet the environmental requirements listed in Table 14. The distribution of wastewaters between WWTU(SITE) and WWTU(PLANT) is governed by their costs because the maximum allowable concentrations are similar for both sinks. In other words, it is always preferred to discharge wastewater to the former unless the full capacity has been reached.

The least-consumption WUTN in Figure 13 can be obtained on the basis of F^W. In this case, a saving of 7% (from 765.5 to 712 tons/h) in fresh water can be achieved. However, the decrease in total throughput

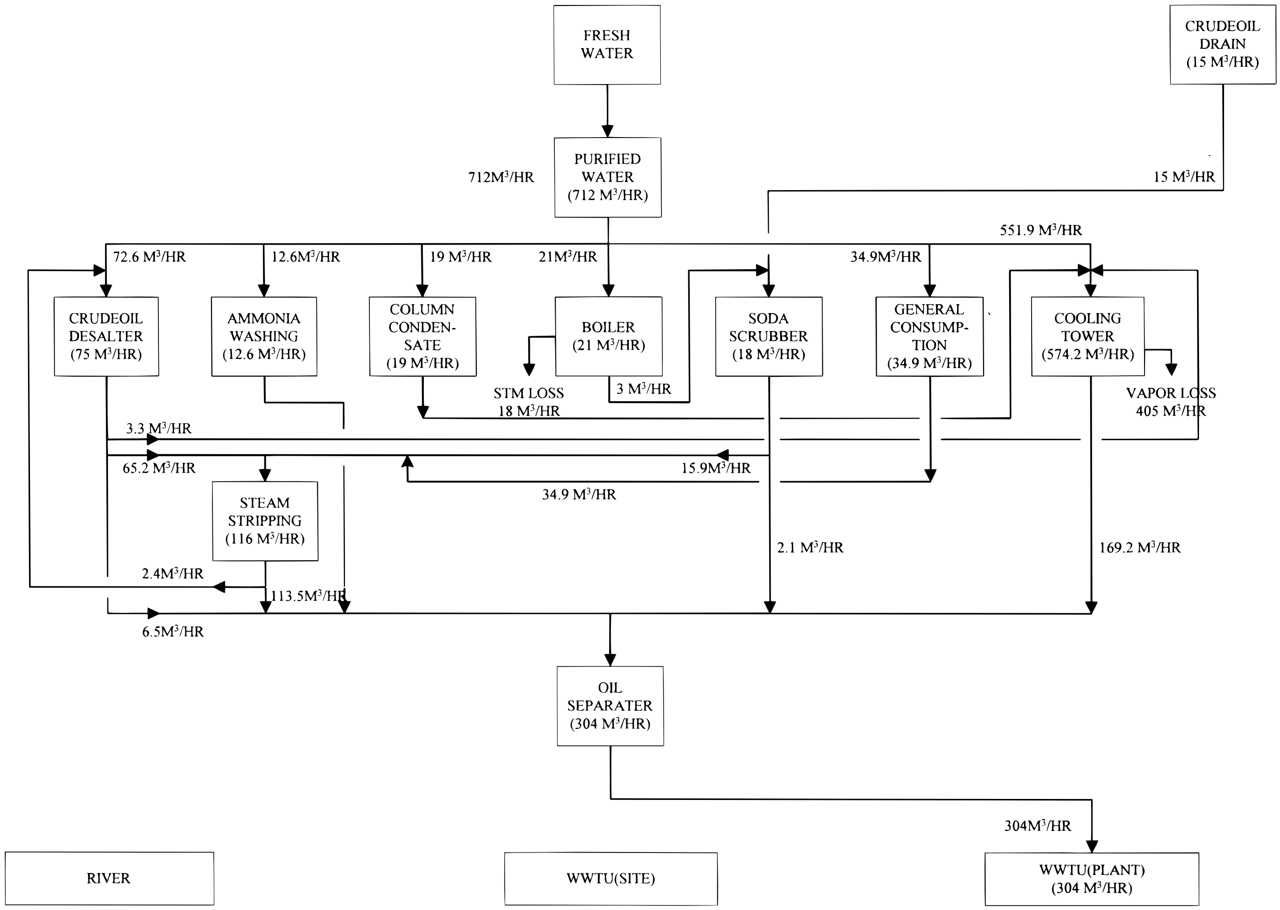

Figure 13. Block diagram of a least-consumption WUTN in the refinery, case 1: API-treated water is not reused.

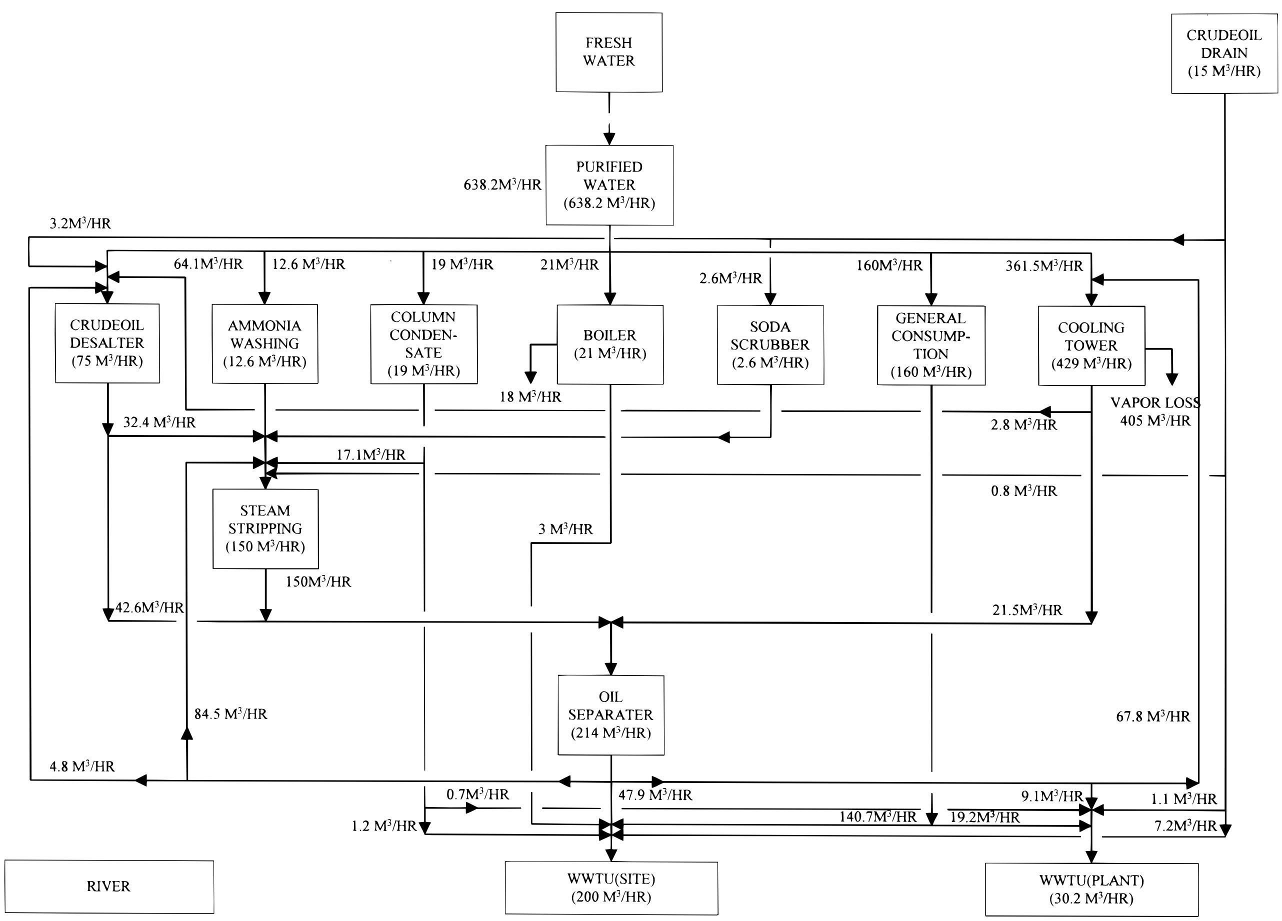

Figure 14. Block diagram of a cost-optimal WUTN in the refinery, case 2: API-treated water is reused.

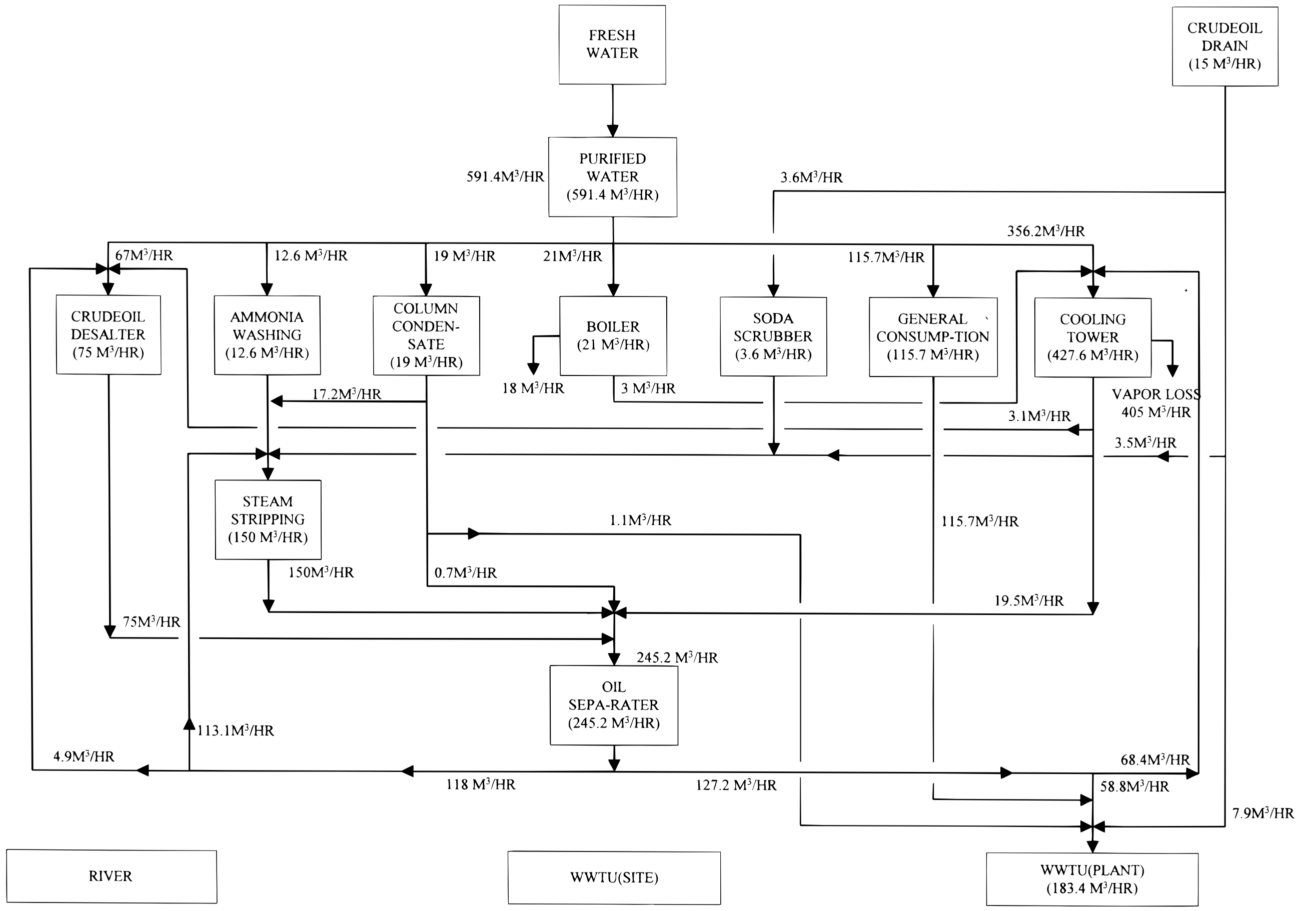

Figure 15. Block diagram of a least-consumption WUTN in the refinery, case 2: API-treated water is reused.

(from 1232 to 1174.7 tons/h) is not significant. The design principles adopted in Figure 13 for optimizing water usage can be summarized as follows. First of all, it is obvious that the secondary waters must be utilized as much as possible. Second, the quality of waters used in water-using units should be enhanced so that the resulting wastewaters are clean enough for downstream units. Third, it is desirable to promote regeneration, reuse, and recycle without discharging wastewaters to the sinks. Finally, all of the wastewaters are sent to WWTU(PLANT) because its requirements are the least stringent and cost is not our emphasis in design.

If the concerns about the API-treated water are actually ungrounded, then the first additional constraint mentioned above should be dropped. The mathematical program can then be solved again accordingly. The resulting cost-optimal and least-consumption WUTNs are presented in Figures 14 and 15, respectively. It can be seen that still better results can be identified. In the former case, not only F^C can be lowered by 30% (from 1947.0 to 1343.8) but also the fresh water consumption rate can be decreased to 638.2 tons/h. On the other hand, the minimum fresh-water flow rate in the latter case is 591.4 tons/h, and the corresponding value of F^C is 1436.5.

Conclusions

A mathematical programming model for finding the minimum fresh-water consumption rate and wastewater-treatment capacity is proposed in this paper. In comparison with the previous approaches, the proposed method is more reliable, more accurate, and more efficient in constructing the WUTNs. In addition, because process-water usage, utility-water consumption, and wastewater treatment can be analyzed under the same framework, the resulting designs should be more comprehensive. Not only different features of various units in WUTN can be incorporated but also the potential benefits of adopting more complex flow configurations, such as repeated treatment units, multiple sources, and sinks, can be easily evaluated with the proposed model. Finally, it should be noted that this method has been successfully applied to two petrochemical plants in Taiwan.

Nomenclature

B^X_{ik} = concentration of solute k at the inlet of the ith water-using unit

B^Y_{jk} = concentration of solute k at the inlet of the jth water-treatment unit

C^X_{ik} = concentration of solute k at the outlet of the ith water-using unit

C^Y_{jk} = concentration of solute k at the outlet of the jth water-treatment unit

D^X_{ik} = concentration of solute k in the loss stream of the ith water-using unit

D^Y_{jk} = concentration of solute k in the loss stream of the jth water-treatment unit

F^C = objective function representing a measure of the total operating cost

F^W = objective function representing the total rate of water consumption or wastewater generation

L_j = water loss in the jth water-treatment unit

M_{jk} = mass load in the jth water-treatment unit

W_p^{P} = consumption rate of the pth primary water
X_i, $\bar{X}_i$ = water flow rate at the inlet and outlet of the ith water-using unit
Y_j, $\bar{Y}_j$ = water flow rate at the inlet and outlet of the jth water-treatment unit
Z_a^{A} = discharge rate to the ath type A sink
Z_b^{B} = discharge rate to the bth type B sink
$Z_{\mathrm{T}}^{\mathrm{C}}$ = combined flow rate of water losses from all water-treatment units
$Z_{\mathrm{U}}^{\mathrm{C}}$ = combined flow rate of water losses from all water-using units

Greek Letters

β_{ik}^{X} = maximum allowable concentration of solute k at the inlet of water-using unit i
β_{jk}^{Y} = maximum allowable concentration of solute k at the inlet of water-treatment unit j
γ_{ik}^{X} = maximum allowable concentration of solute k at the outlet of water-using unit i
η_j = upper bound of throughput in water-treatment unit j
$\lambda_{ik}^{\mathrm{X}}$ = constant concentration at the outlet of water-using unit i
$\lambda_{jk}^{\mathrm{Y}}$ = constant concentration at the outlet of water-treatment unit j
μ_{ik} = mass load of solute k in the ith water-using unit
ν_i = operation loss of the ith water-using unit
ϕ_j = fraction of loss water in water-treatment unit j
ψ_{jk} = removal ratio of solute k in water-treatment unit j
ω_u^{X}, ω_t^{Y}, ω_b^{Z} = weighting factors

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Received for review January 20, 1999
Revised manuscript received April 20, 1999
Accepted April 29, 1999

IE990043S