Two-Step Optimization Approach for Design of A Total Water System

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Two-Step Optimization Approach for Design of A Total Water System

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The development of the two-step optimization approach, as seen in Part 1 of the paper, can then be extended to a total water system. The total water system comprises two subsystems: namely, water-using units and wastewater treatment system. In this paper, the proposed approach utilizes mixed integer linear programming (MILP) and nonlinear programming (NLP) in the two-step optimization approach to generate multiple optimum solutions, called "class of good solutions", for the total water system design problem. A case study from the literature is used to illustrate the proposed approach, and comparisons with the results from the current techniques were then made to demonstrate the proposed method's strength.

Introduction

The increasing cost of freshwater supply, wastewater treatment, and the stringent environmental regulations have driven industrial plants to become more efficient in their use of water. Of many approaches to make the water use efficient, the concept of water reuse, regeneration, and recycle has been widely accepted by the process industries. This concept is not only applied at several water-using operations in the plant but also at the total water system consisting of water-using and wastewater treatment operations. In the case of the total water system, the challenge is to meet both the process requirements and the environmental regulations simultaneously while cost effectively pursuing water or wastewater minimization initiatives. This paper will address this issue by proposing a practical approach to generate family of practical options for water or wastewater minimization projects.

As expected, the design of total water system requires large mathematical formulations constructed in nonlinear programming (NLP) for a fixed number of operations. Solving an NLP problem requires good initializations; otherwise, in many cases, it will end up with no solution. The mathematical optimization approach, such as NLP, for solving the water or wastewater minimization problems has been reported in the literature since the 1980s. The early work was a problem to reduce freshwater consumption in a petroleum refinery in 1980.[1] Through extensive research, it was concluded that there was an even bigger opportunity to reduce large quantities of freshwater consumed and wastewater discharged when a system involving water-using operations and a wastewater treatment system is considered, rather than to focus on a water-using operation alone. Other researchers[2] agreed with this observation. The petroleum case study[1] involved three contaminants, three water-using operations, and three wastewater treatment operations. The problem was solved by using a complex method after transforming the nonlinearities into a sequence of linear functions without inequality constraints by employing a penalty function.

In the next decades, works in mass-exchange operations[3] and water pinch analysis[4–6] established a similar concept with heat exchanger networks (HEN) for freshwater and wastewater minimization. Concerning a total water system that involves water-using operations and a wastewater treatment system, a graphical approach was presented to target minimum freshwater consumption as well as minimum wastewater produced.[7] Later, interactions between water-using, regeneration, and wastewater treatment operations were explored to improve the design of water networks.[8] This exploration involved grouping and migrating of the operations. The aforementioned methods were developed in graphical manner to provide designers with significant insights into the process. Unfortunately, these graphical approaches were mainly based on an assumption of using only a single contaminant. Even though these graphical approaches were adopted to solve multiple contaminants problems, those approaches were very cumbersome and tedious to be applied.

Another approach to solve the complex multiple contaminants problem is an optimization of mathematical programming. The water system design involving water-using operations and wastewater treatment units were formulated in mixed integer nonlinear programming (MINLP).[9–13] The complex mathematical programming problems were decomposed into a sequence of mixed integer linear programming (MILP) problems to approximate the optimal solution, and the problems were solved iteratively. At the final step, the optimized problems were further optimized by using NLP with fixed total water system.[9–11] Other authors claimed to have improved this method by simplifying the mathematical models, thus, reducing the calculation time.[12,13] The simplification was that the mathematical models for mass-exchange networks to calculate the number of trays were removed. This of course reduced the complexity of the problems. Then, instead of using NLP for the final optimization, these authors utilized MINLP to ensure that the optimum configuration was generated.[12,13] Instead of formulating the problems into MINLP, others[14] constructed NLP for a fixed number of water-using operations and wastewater treatment units. They used reasonable initialization points to solve the problem. Nonetheless, mathematical formulations for total water systems involving water-using operations and wastewater treatment units are nonconvex nonlinear problems. Thus, as the complexity arises in the formulations, the solution is rather complicated to generate, and, furthermore, there is no guarantee that the generated solution is a global optimum solution. This issue of global optimization has attracted many researchers to this date.[2]

Previous works on the total water system design showed a magnificent breakthrough for the development of the water

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reuse, regeneration, and recycle concept. The graphical approach provided valuable insights of the water system while the mathematical programming managed to solve large and complex water problems resulting in either local or global optimum solutions. Nonetheless, most of the current work in water minimization modeling only focused on how to achieve the global optimum solution, which is primarily driven by economics. It is no doubt that the global optimum can be achieved, but such a solution suffers from the lack of practical design concerns such as the considerations of piping sizes and piping complexity, geographical constraints, safety, operability, and forbidden or compulsory piping interconnections. The mathematical formulations of MINLP by some authors[9–13] have successfully addressed these considerations. However, their method still failed to get multiple solutions because of their intention to get an optimum solution with the given practical consideration. Their methods could generate multiple solutions in some ways, especially when multiple initialization points were provided. Nonetheless, they did not demonstrate this feature adequately in their work. Having multiple solutions enables a designer to choose which solution really meets their further requirements, especially when certain considerations such as safety and operability problems or perhaps company preferences cannot be modeled in mathematical relationships.

This paper proposes an alternative solution strategy for solving total water system design problem by utilizing MILP and NLP in a two-step optimization approach. The approach has the advantages of the capability to produce multiple solutions simultaneously and to consider practical considerations, as well as to provide users with the ability to control the water network during the optimization process. The approach consists of two steps, namely, structural targeting step and parametric optimization step. The structural targeting step utilizes MILP to get more than one optimum total water systems which still considers practical constraints and users' preferences, while the parametric optimization step utilizes NLP to optimize the parametric values for each of the optimum total water systems. At the end, users can assess all solution options and pick out the one that meets their criteria.

Problem Decomposition

The two-step optimization approach seeks the optimum water structures with the considerations of practical constraints by utilizing MILP formulations. The benefit of having MILP for the structural optimization step is that the MILP formulations can be solved globally, which ensures that the resulted water structures are the global solutions. Another usage of MILP formulation in this approach is its inherent feature of allowing user to control the piping interconnections. Then, the NLP solver is used to generate the optimum parametric values for each of the optimum water structures previously obtained from MILP optimization.

Total water system design requires large and complex mathematical formulations to be optimized. As previously shown by other researchers, this system can only be formulated in either MINLP[9–13] or NLP.[1,2,14] Therefore, to formulate the total water system into MILP formulations, the system is decomposed into three main subsystems. The first subsystem is the water reuse subsystem where all reuse opportunities are explored. The second subsystem is the placement of the regeneration unit, where the water network(s) from the first subsystem is chosen as the base network for regeneration unit. The first and the second subsystems are similar to the one shown in part 1 of this paper.[17] The third subsystem is wastewater treatment where

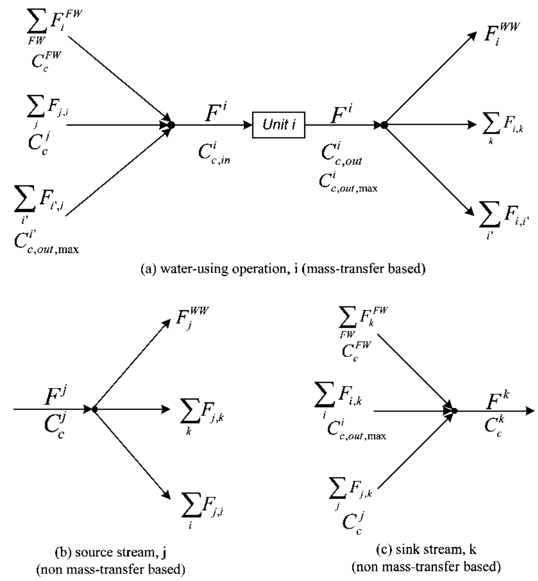

Figure 1. Superstructure of water-using operations showing all possible reuse options.

wastewater streams from the first and second subsystems are taken as a basis for optimizing the associated treatment units.

Water Reuse Subsystem

The subsystem explores, in the form of superstructures (Figure 1), water reuse opportunities to reduce freshwater consumption and, hence, wastewater discharge. The search for water reuse opportunities is important before a regeneration unit, if any, can be considered. The most logical step is to start by searching for a simple piping modification for water reuse, say one pipework modification connecting from a water outlet in a water-using operation (supply or source) to a water inlet of *another* water-using operation (sink). Then, more piping modifications can be added to quantify how much freshwater can be reduced further. The two-step optimization approach of MILP-NLP is utilized to explore all these reuse possibilities. MILP formulations allow the user to manually control the development of water network structures while considering the aforementioned practical aspects. NLP formulations provide the user with the optimum parametric values for each of the water networks generated from the MILP solutions.

Structural Targeting Step. The structural targeting step is meant to explore every possible reuse structure of the water network. In this MILP approach, two common types of water-using operations, mass-transfer and non-mass-transfer based, are addressed in this mathematical formulation. The superstructure concerning these water-using operations is shown in Figure 1.

A number of freshwater sources and water reuse streams from any water-using operation are mixed at the inlet of each water-using operation. The outlet stream of each water-using unit operation is split and connected to every possible connection of water reuse that can be made.

Each water-using operation is supplied with a certain quantity and quality of water. Mass-transfer based water-using operations are supplied by their corresponding limiting water flowrate and maximum inlet contaminant concentration.[15] The contaminants in the outlet streams of mass-transfer based water-using operations are assumed to reach their maximum outlet contaminant concentration.[16] The inlet and outlet streams of non-mass-transfer based water-using operations have their own fixed water flowrate as well as maximum inlet and outlet contaminant concentration. Water-using operations with the mass-transfer model are denoted with i (where $i \in I$), whereas the non-mass-transfer model denotes j for source streams (where $j \in J$) and k for sink streams (where $k \in K$), and contaminants are denoted with c (where $c \in C$). The mathematical relationships at the mixing point are as follows:

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} + \sum_{i'} F_{i'i} + \sum_{j} F_{j,i} = F^i \qquad \forall\, i \in I, i \neq i' \quad (1)$$

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_{i'} F_{i'i} C_{c,\mathrm{out,max}}^{i'} + \sum_{j} F_{j,i} C_c^{j} = F^i C_{c,\mathrm{in}}^{i} \qquad \forall\, c \in C, i \in I, i \neq i' \quad (2)$$

$$\sum_{\mathrm{FW}} F_k^{\mathrm{FW}} + \sum_{i} F_{i,k} + \sum_{j} F_{j,k} = F^k \qquad \forall\, k \in K \quad (3)$$

$$\sum_{\mathrm{FW}} F_k^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_{i} F_{i,k} C_{c,\mathrm{out,max}}^{i} + \sum_{j} F_{j,k} C_c^{j} \le F^k C_c^{k} \qquad \forall\, c \in C, k \in K \quad (4)$$

where F_i^{FW} and F_k^{FW} are the freshwater flowrate supplying mass-transfer based water-using operations and sink streams of water-using operations, respectively. $F_{i',i}$, $F_{i,k}$, $F_{j,i}$, and $F_{j,k}$ are water reuse streams from water-using operations to other water-using operations. C_c^{FW}, $C_{c,\mathrm{in}}^{i}$, $C_{c,\mathrm{out,max}}^{i}$, C_c^{j}, and C_c^{k} are concentrations of contaminants for each corresponding stream. In this paper, the presence of local recycle (water recycle within the same unit of the water-using operation), which is practically not acceptable to most process industries due to a possible accumulation of certain contaminants in this recycle loop over the time, is not considered.

Contaminant balances throughout the mass-transfer based water-using operations are defined as

$$F^i (C_{c,\mathrm{out}}^{i} - C_{c,\mathrm{in}}^{i}) = \Delta m_c^i \qquad \forall\, i \in I \quad (5)$$

where Δm_c^i is the fixed mass load of contaminant transferred in the operations. On the basis of the assumption that all contaminants reach their maximum outlet concentrations, the following equations can be derived:

$$C_{c,\mathrm{out,max}}^{i} \ge C_{c,\mathrm{out}}^{i} \qquad \forall\, c \in C \quad (6)$$

$$F^i C_{c,\mathrm{out,max}}^{i} - F^i C_{c.\mathrm{in}}^{i} \ge \Delta m_c^i \qquad \forall\, i \in I \quad (7)$$

Combining eqs 1 and 2 with eq 7 gives

$$\left[\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} + \sum_{i'} F_{ii} + \sum_{j} F_{j,i}\right] C_{c,\mathrm{out,max}}^{i} - \left[\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_{i'} F_{i'i} C_{c,\mathrm{out,max}}^{i'} + \sum_{j} F_{j,i} C_c^{j}\right] \ge \Delta m_c^i \qquad \forall\, c \in C, i \in I, i \neq i' \quad (8)$$

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} (C_{c,\mathrm{out,max}}^{i} - C_c^{\mathrm{FW}}) + \sum_{i'} F_{i'i} (C_{c,\mathrm{out,max}}^{i} - C_{c,\mathrm{out,max}}^{i'}) + \sum_{j} F_{j,i} (C_{c,\mathrm{out,max}}^{i} - C_c^{j}) \ge \Delta m_c^i \qquad \forall\, c \in C, i \in I, i \neq i' \quad (9)$$

At the splitter point for both types of water-using operations, each of the outlet streams is split and connected to any possible water reuse connections in the water network.

$$F^i = \sum_{i'} F_{i,i'} + \sum_{k} F_{i,k} + F_i^{\mathrm{WW}} \qquad \forall\, i \in I, i \neq i' \quad (10)$$

$$F_j = \sum_{i} F_{j,i} + \sum_{k} F_{j,k} + F_j^{\mathrm{WW}} \qquad \forall\, j \in J \quad (11)$$

Binary variables (z) are introduced to control the development of the water network as well as to explore every water reuse opportunity while considering the practical aspects of the designs.

$$M z^{ii'} \le F_{i,i'} \le F^i z^{ii'} \qquad \forall\, i \in I, i \neq i' \quad (12)$$

$$M z^{ik} \le F_{i,k} \le F^i z^{ik} \qquad \forall\, k \in K \quad (13)$$

$$M z^{ji} \le F_{j,i} \le F^j z^{ji} \qquad \forall\, i \in I \quad (14)$$

$$M z^{jk} \le F_{j,k} \le F^j z^{jk} \qquad \forall\, k \in K \quad (15)$$

$$\sum_{i'} z_{i,i'} + \sum_{j} z_{i,j} + \sum_{i} z_{j,i} + \sum_{k} z_{j,k} = N \quad (16)$$

where M is the lowest acceptable and economical flowrate flowing through the pipes and N is the number of allowed water reuse streams permitted. Specifically, N is the number of piping modifications required as specified by the users, which defines the level of piping complexity. Thus, the higher the value of N, the more complicated the water network will be. Defining the number of reuse streams connected to each water-using operation can also be used to control the level of piping complexity.

$$\sum_{i'} z^{i'i} + \sum_{j} z^{ji} = P \qquad \forall\, i \in I, i \neq i' \quad (17)$$

$$\sum_{i} z^{ik} + \sum_{j} z^{jk} = Q \qquad \forall\, k \in K \quad (18)$$

where P and Q are the highest amount of water reuse streams allowable to be attached to the operations.

The objective function is to reduce the total freshwater consumption, as shown below:

$$F_{\mathrm{total}}^{\mathrm{FW}} = \sum_{i} F_i^{\mathrm{FW}} + \sum_{k} F_k^{\mathrm{FW}} \quad (19)$$

Thus, for a given number of piping modifications that feature a specific number of water reuse streams, one can find this structure that minimizes the total freshwater consumption. As expected, the total freshwater consumption can be reduced further when more piping modifications are added. At the end, the users should have many water reuse networks with several levels of piping complexity as the basis for the next step. Of course, the basis for the selection, among others, will consider the incremental benefits of additional water savings for additional piping modifications required for water reuse. Thus, the structural optimization step allows the users to construct as many options as possible of water reuse networks toward achieving minimum freshwater consumption while controlling the level of piping complexity.

Parametric Optimization Step. The parametric optimization step is intended to optimize the parametric values for each of the previously obtained water reuse networks using NLP. In this step, the optimized water reuse networks from the structural targeting step are held fixed. On the basis of these water reuse networks, mathematical relationships are constructed as follows:

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} + \sum_{i'} F_{i'i} + \sum_{j} F_{j,i} = F^i \qquad \forall\, i \in I, i \neq i' \quad (20)$$

$$\sum_{\mathrm{FW}} F_k^{\mathrm{FW}} + \sum_{i} F_{i,k} + \sum_{j} F_{j,k} = F^k \qquad \forall\, k \in K \quad (21)$$

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_{i'} F_{i'i} C_{c,\mathrm{out}}^{i'} + \sum_{j} F_{j,i} C_c^{j} = F^i C_{c,\mathrm{in}}^{i} \qquad \forall\, c \in C, i \in I, i \neq i' \quad (22)$$

$$\sum_{\mathrm{FW}} F_k^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_i F_{i,k} C_{c,\mathrm{out}}^i + \sum_j F_{j,k} C_c^j \le F^k C_c^k \qquad \forall\, c \in C, k \in K \quad (23)$$

$$C_{c,\mathrm{in}}^i \le C_{c,\mathrm{in,max}}^i \qquad \forall\, c \in C, i \in I \quad (24)$$

The mathematical models for mass-transfer based operations (eq 5) together with the split streams from both water-using operations (eqs 10 and 11) can be added to this NLP formulation.

These mathematical relationships exhibit nonlinearities, especially at the mixing point for mass-transfer based water-using operations. These nonlinearities results in a local optimum solution which is inherent to all NLP solvers. The optimum solution from NLP solvers depends strongly on the initialization provided by the user. In this work, the structural optimization step provides such an initialization.

Then, for each water network obtained in the structural targeting step, the parametric values are optimized using the same objective function of reducing the total freshwater consumption (eq 19). At the end, the users will have a multiple water reuse network as the basis for the subsequent placement of the regeneration unit or wastewater treatment subsystem.

Placement of the Regeneration Unit

Having explored all the water reuse possibilities, a water regeneration unit can be considered to further reduce the total freshwater consumption. The regeneration unit must be placed on the optimized water reuse network having the highest level of piping complexity where no water reuse opportunity can be taken. The two-step optimization approach can be applied in this water regeneration scheme as well.

Structural Targeting Step. The structural targeting step for this water regeneration scheme is to identify water-using operations that can be supplied by the regenerated water and streams to be regenerated to satisfy the identified operations. This identification will be different when dealing with the regeneration unit characterized by fixed removal ratio or by fixed outlet contaminant concentration.

The regeneration unit characterized by fixed removal ratio produces nonlinear mathematical relationships at the mixing point of the unit. To overcome this, the amount of wastewater that needs to be regenerated must be assumed first. The identified water-using operations that can be supplied by the regenerated water provide this information. This amount of regenerated water is taken as the amount of wastewater supplied to the regeneration unit where there is no water loss in the regeneration unit. Then, wastewater streams in the chosen water reused networks are listed in ascending order of contaminant concentration. The concentration order is established on the basis of the specification of the regeneration unit involved. For example, if the regeneration unit can only remove contaminant A or have the highest removal ratio of contaminant A rather than the other contaminants, then the wastewater streams are ordered on the basis of the concentration of contaminant A. The "cleaner" wastewater stream is put on the top of the list, while the "dirtiest" wastewater is put last on the list. The amount of wastewater regenerated in the regeneration unit is satisfied by the "cleaner" wastewater first and then by the next rank of the wastewater concentration list. This approach is considered because the "cleaner" wastewater streams will produce "cleaner" regenerated water due to the fixed removal ratio. This condition will bring higher opportunity of the regenerated water for being reused further. This approach is shown in Figure 2.

Figure 2 shows that the amount of regenerated water depends on the water-using operations that can be supplied by the regenerated water. These water-using operations represent the new sink streams with their associated flowrate and inlet concentration, while the regenerated water is considered as the new source stream.

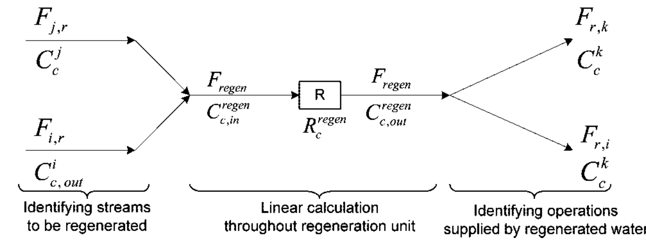

Figure 2. Formulating linear equations throughout regeneration unit.

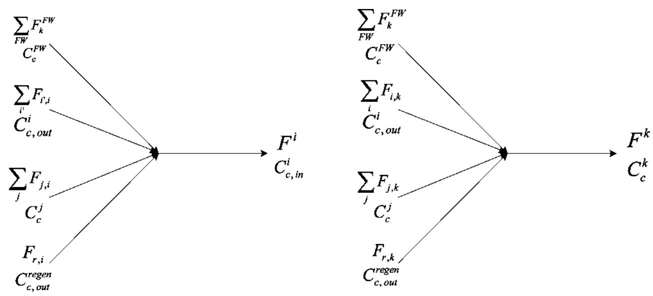

Figure 3. Extended superstructure involving new source and sink streams.

$$\sum_k F_{r,k} + \sum_i F_{r,i} = F_{\mathrm{regen}} = \sum_j F_{j,r} + \sum_i F_{i,r} \quad (25)$$

where $F_{r,k}$ and $F_{r,i}$ represent the amount of regenerated water that can be supplied to the water-using operations, F_{regen} represents the amount of regenerated water throughout the regeneration unit, $F_{j,r}$ and $F_{i,r}$ represent the amount of wastewater assumed to be regenerated to fulfill the water requirement amount for the water-using operations.

The contaminant balance at the inlet of regeneration unit can be calculated on the basis of the flowrate and concentration of wastewater streams assumed to be regenerated.

$$\sum_j (F_{j,r} C_c^j) + \sum_i (F_{i,r} C_{c,\mathrm{out}}^i) = F_{\mathrm{regen}} C_{c,\mathrm{in}}^{\mathrm{regen}} \qquad \forall\, c \in C \quad (26)$$

For a specified removal ratio, the outlet concentration can then be calculated as follows:

$$C_{c,\mathrm{out}}^{\mathrm{regen}} = C_{c,\mathrm{in}}^{\mathrm{regen}} (1 - R_c^{\mathrm{regen}}) \qquad \forall\, c \in C \quad (27)$$

Equation 30 provides the outlet concentration of the regenerated water. This regenerated water becomes the new water sources. The outlet stream of the regeneration unit is split to operations that can be supplied with regenerated water.

$$F_{\mathrm{regen}} = \sum_k F_{r,k} + \sum_i F_{r,i} \quad (28)$$

When the regeneration unit is characterized by its fixed outlet concentration ($C_{c,\mathrm{out}}^{\mathrm{regen}}$), any inlet contaminant concentration will still produce the same outlet contaminant concentration. Therefore, the mass balance calculation at the inlet of the regeneration unit can be removed. The amount of regenerated water is a variable, but the outlet concentration is a fixed parameter. The regenerated water stream is split ($F_{r,k}$ and $F_{r,i}$) and attached to water-using operations on the chosen water reuse network.

Figure 3 shows an extended superstructure involving the identified water-using operations with its associated freshwater stream, water reuse streams, and the regenerated water. Mathematical relationships regarding this extended superstructure can be shown as follows:

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} + \sum_i F_{i,i} + \sum_j F_{j,i} + F_{r,i} = F^i \qquad \forall\, i \in I, i \neq i' \tag{29}$$

$$F_k^{\mathrm{FW}} + \sum_i F_{i,k} + \sum_j F_{j,k} + F_{r,k} = F^k \qquad \forall\, k \in K \tag{30}$$

$$\sum_{\mathrm{FW}} F_i^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_i F_{i,i} C_{c,\mathrm{out}}^{i'} + \sum_j F_{j,i} C_c^j + F_{r,i} C_{c,\mathrm{out}}^{\mathrm{regen}} = F^i C_{c,\mathrm{in}}^i \qquad \forall\, c \in C, i \in I, i \neq i' \tag{31}$$

$$F_k^{\mathrm{FW}} C_c^{\mathrm{FW}} + \sum_i F_{i,i} C_{c,\mathrm{out,max}}^{i'} + \sum_j F_{j,i} C_c^j + F_{r,i} C_{c,\mathrm{out}}^{\mathrm{regen}} = F_k C_c^k \qquad \forall\, c \in C, k \in K \tag{32}$$

The amount of water reuse streams for the regenerated water can be controlled by using binary variables (z),

$$Mz^{rk} \le F_{r,k} \le F_{\mathrm{regen}} z^{rk} \qquad \forall\, k \in K \tag{33}$$

$$Mz^{ri} \le F_{r,i} \le F_{\mathrm{regen}} z^{ri} \qquad \forall\, i \in I \tag{34}$$

Then, the new sink streams are to be optimized using MILP with the objective function of reducing their associated freshwater consumption. The users should have the ability to control the number of water reuses/recycles of the regenerated water in this scheme by considering possible constraints.

Parametric Optimization Step. Having obtained water regeneration structures, this extended structure is combined with the previous water reuse networks. The (NLP)[14] mathematical relationships are created, and the water regeneration networks from the structural targeting step are taken as the initializations. The complete superstructure for this NLP is shown in Figure 4. Some of mathematical relationships for NLP formulations are similar to the previous equations, especially those involving water-using operations such as eqs 5, 24, and 29–32. Outlet streams of water-using operations are split the the reuse and to the regeneration unit as shown below:

$$F^i = \sum_{i'} F_{i,i'} + \sum_k F_{i,k} + F_{i,r} + F_i^{\mathrm{WW}} \qquad \forall\, i \in I \tag{35}$$

$$F_j = \sum_i F_{j,i} + \sum_k F_{j,k} + F_{j,r} + F_j^{\mathrm{WW}} \qquad \forall\, j \in J \tag{36}$$

$$\sum_i F_{i,r} + \sum_j F_{j,r} = F_{\mathrm{regen}} \tag{37}$$

For the regeneration unit characterized by a fixed removal ratio, the material balance at the mixing point of the regeneration unit is similar to eq 26, while the outlet concentration is calculated according to eq 27. Thus, the outlet stream of the regeneration unit is formulated as follows:

$$F_{\mathrm{regen}} = \sum_i F_{r,i} + \sum_k F_{r,k} + F_r^{\mathrm{WW}} \tag{38}$$

The objective function is still to minimize the total freshwater consumption as shown in eq 19.

Wastewater Treatment Subsystem

The basic method of this approach is adapted from basic network superstructures (BNS) for a given set of wastewater treatment units.[18] In this approach, for a given set of wastewater treatment units, those units are arranged or sequenced into a set of $n!$ BNS. However, some of the treatment units may have certain requirements of operating conditions which require or forbid those units to be in certain sequences. In other words, some treatment units should be placed at the upstream or downstream of other treatment units. This in turn simplifies the BNS.

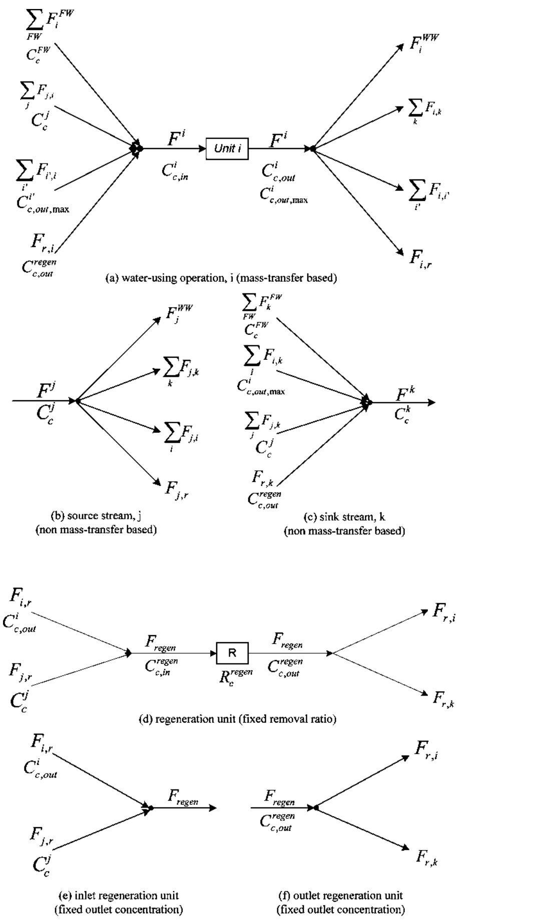

Figure 4. Complete superstructure for water-using operations and the regeneration unit.

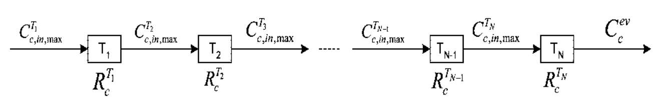

Figure 5. Maximum allowable inlet concentrations.

Environmental regulations often limit the concentration of certain chemical species or contaminants before the wastewater stream being discharged to the environment. In defining the mathematical expressions for the wastewater treatment units, it is easier to characterize the units with fixed removal ratios, as described earlier in the water-using subsystem. With the given maximum allowable concentration discharge limit for each contaminant (C_c^{env}), for each set of BNS, "maximum allowable inlet concentrations ($C_{c,\mathrm{in,max}}^{\mathrm{T}N}$)" for each preceded treatment unit is calculated backward from the discharge points to the first treatment unit in each BNS. This maximum allowable inlet concentration is shown in Figure 5.

These maximum allowable inlet concentrations are redefined as "maximum allowable mixing concentrations", as shown in Figure 6. The concentration of mixing all wastewater streams with the outlet of the preceding treatment units must not exceed the maximum allowable mixing concentrations. This is to ensure

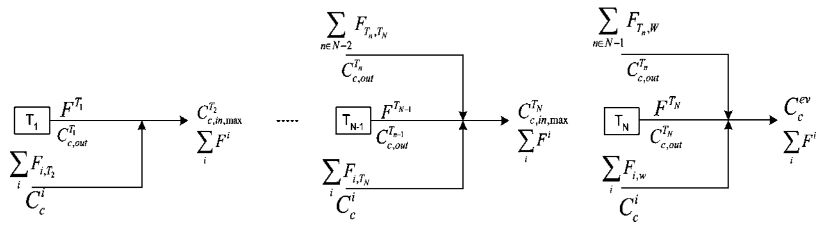

Figure 6. Maximum allowable mixing concentrations ensures the environmental limit is met.

that when all of the wastewater streams, including the one leaving from the preceding treatment units, are mixed, the subsequent treatment unit will have no constraint of treating the waste to meet the environmental discharge limit.

Having established the maximum allowable mixing concentrations for each wastewater treatment unit in every BNS of the wastewater treatment system, one can apply the two-step optimization approach.

Structural Targeting Step. The structural targeting step is aimed at providing manual control for the users to have many options in the wastewater treatment system. Having calculated those maximum allowable mixing concentrations in the backward direction from discharge, one can then develop mathematical relationships in the forward direction from the first treatment unit toward discharge for every BNS. The formulations are developed for each treatment unit in every sequence of wastewater treatment units (in every BNS).

Each wastewater stream is split to supply the first and the second treatment unit in every sequence of the wastewater treatment units or BNS:

$$F^i = F_{i,\mathrm{T1}} + F_{i,\mathrm{T2}} \qquad \forall\, i \in I \tag{39}$$

Then, the water balance for the first treatment unit can be calculated as follows:

$$F^{\mathrm{T1}} = \sum_i F_{i,\mathrm{T1}} \tag{40}$$

$$F^{\mathrm{T1}} C_{c,\mathrm{in}}^{\mathrm{T1}} = \sum_i F_{i,\mathrm{T1}} C_c^i \qquad \forall\, c \in C \tag{41}$$

$$C_{c,\mathrm{out}}^{\mathrm{T1}} = C_{c,\mathrm{in}}^{\mathrm{T1}} (1 - R_c^{\mathrm{T1}}) \qquad \forall\, c \in C \tag{42}$$

As highlighted in the water-using subsystem, eq 41 is the source of nonconvexity in the formulation due to the multiplication of variables. To avoid this nonconvexity, eqs 41 and 42 are modified to

$$M_{c,\mathrm{in}}^{\mathrm{T1}} = \sum_i F_{i,\mathrm{T1}} C_c^i \qquad \forall\, c \in C \tag{43}$$

$$M_{c,\mathrm{out}}^{\mathrm{T1}} = M_{c,\mathrm{in}}^{\mathrm{T1}} (1 - R_c^{\mathrm{T1}}) \qquad \forall\, c \in C \tag{44}$$

where $M_{c,\mathrm{in}}^{\mathrm{T1}}$ and $M_{c,\mathrm{out}}^{\mathrm{T1}}$ are load of contaminants for the inlet and outlet of the first treatment unit in the sequence, respectively. However, if there is a maximum inlet concentration allowable for each treatment unit, the following equations can be added:

$$\sum_i F_{i,\mathrm{T1}} C_c^i \le F_{\mathrm{T1}} C_{c,\mathrm{in,max}}^{\mathrm{T1}} \qquad \forall\, c \in C \tag{45}$$

At the outlet of the first treatment unit, there is a "maximum allowable mixing concentration" for each contaminant. This condition has to be met in case all of the wastewater needs to be treated in the second treatment unit in each sequence of wastewater treatment units.

$$\sum_i F_{i,\mathrm{T2}} C_c^i + M_{c,\mathrm{out}}^{\mathrm{T1}} \le C_{c,\mathrm{in,max}}^{\mathrm{T2}} \left[\sum_i F^i \right] \qquad \forall\, c \in C \tag{46}$$

Binary variables (z) are introduced to specify the minimum and maximum water flowrates as well as to control the piping configurations.

$$M z^{i\,\mathrm{T1}} \le F_{i,\mathrm{T1}} \le F^i z^{i\,\mathrm{T1}} \tag{47}$$

$$M z^{i\,\mathrm{T2}} \le F_{i,\mathrm{T2}} \le F^i z^{i\,\mathrm{T2}} \tag{48}$$

where M is the minimum water flowrate permitted to be flowing through the pipes. Controlling the piping configurations is achieved by setting the number of streams to be combined and treated for one treatment unit and the number of streams to be bypassed to the next treatment.

$$\sum_i z^{i\,\mathrm{T1}} = A^{\mathrm{T1}} \tag{49}$$

$$\sum_i z^{i\,\mathrm{T2}} = A^{\mathrm{T2}} \tag{50}$$

where A is a value that limits the mixing of streams at the inlet of the first treatment (T1) and the second treatment unit (T2), respectively.

The objective function is to minimize the flowrate treated in the first treatment unit.

$$\mathrm{obj} = \min F^{\mathrm{T1}} \tag{51}$$

Similarly, the same approach can be applied to the second treatment in the sequence of wastewater treatment units. The remaining flowrate of the wastewater streams and the outlet flowrate from the first treatment are brought to the optimization of the second treatment unit in the same sequence. The structure obtained from this optimization is kept throughout this sequence optimization. The outlet concentration of the first treatment unit needs to be calculated first prior to the formulation of the second treatment unit.

$$C_{c,\mathrm{out}}^{\mathrm{T1}} = \frac{M_{c,\mathrm{out}}^{\mathrm{T1}}}{F^{\mathrm{T1}}} \qquad \forall\, c \in C \tag{52}$$

Then, the mathematical relationships for the optimization of the second treatment unit begin by splitting the remaining streams toward the second and the third treatment units in sequence.

$$F^i = F_{i,\mathrm{T2}} + F_{i,\mathrm{T3}} \qquad \forall\, i \in I \tag{53}$$

$$F^{\mathrm{T1}} = F_{\mathrm{T1,T2}} + F_{\mathrm{T1,T3}} \tag{54}$$

Mathematical relationships in the second treatment unit can then be shown as follows:

$$F^{\mathrm{T2}} = \sum_i F_{i,\mathrm{T2}} + F_{\mathrm{T1,T2}} \tag{55}$$

$$\sum_i F_{i,\mathrm{T2}} C_c^i + F_{\mathrm{T1,T2}} C_{c,\mathrm{out}}^{\mathrm{T1}} \le F^{\mathrm{T2}} C_{c,\mathrm{in,max}}^{\mathrm{T2}} \qquad \forall c \in C \tag{56}$$

$$M_{c,\mathrm{in}}^{\mathrm{T2}} = \sum_i F_{i,\mathrm{T2}} C_c^i + F_{\mathrm{T1,T2}} C_{c,\mathrm{out}}^{\mathrm{T1}} \qquad \forall c \in C \tag{57}$$

$$M_{c,\mathrm{out}}^{\mathrm{T2}} = M_{c,\mathrm{in}}^{\mathrm{T2}} (1 - R_c^{\mathrm{T2}}) \qquad \forall c \in C \tag{58}$$

Limiting the total outlet concentration to its corresponding "maximum allowable mixing concentrations",

$$\sum_i F_{i,\mathrm{T3}} C_c^i + F_{\mathrm{T1,T3}} C_{c,\mathrm{out}}^{\mathrm{T1}} + M_{c,\mathrm{out}}^{\mathrm{T1}} \le C_{c,\mathrm{in,max}}^{\mathrm{T3}} \left[\sum_i F^i \right] \qquad \forall c \in C \tag{59}$$

Binary variables are then introduced:

$$Mz^{i\,\mathrm{T2}} \le F_{i,\mathrm{T2}} \le F^i z^{i\,\mathrm{T2}} \tag{60}$$

$$Mz^{i\,\mathrm{T3}} \le F_{i,\mathrm{T3}} \le F^i z^{i\,\mathrm{T3}} \tag{61}$$

$$Mz^{\mathrm{T1T2}} \le F_{\mathrm{T1,T2}} \le F^{\mathrm{T1}} z^{\mathrm{T1T2}} \tag{62}$$

$$Mz^{\mathrm{T1T3}} \le F_{\mathrm{T1,T3}} \le F^{\mathrm{T1}} z^{\mathrm{T1T3}} \tag{63}$$

$$\sum_i z^{i\,\mathrm{T2}} = A^{\mathrm{T2}} \tag{64}$$

$$\sum_i z^{i\,\mathrm{T3}} = A^{\mathrm{T3}} \tag{65}$$

By using the same objective function of minimizing the treated flowrate in the second treatment unit, the required structures and their parametric values are obtained for the next treatment unit. This type of formulation is repeated *n* times until the last treatment unit for the particular sequence of *n* numbers of wastewater treatment units.

$$F^i = F_{i,\mathrm{T}N} + F_{i,\mathrm{W}} \qquad \forall i \in I \tag{66}$$

$$\sum_{n \in N-1} F^{\mathrm{T}n} = F_{\mathrm{T}n,\mathrm{T}N} + F_{\mathrm{T}n,\mathrm{W}} \tag{67}$$

$$F^{\mathrm{T}N} = \sum_i F_{i,\mathrm{T}N} + \sum_{n \in N-1} F_{\mathrm{T}n,\mathrm{W}} \tag{68}$$

$$\sum_i F_{i,\mathrm{T}N} C_c^i + \sum_{n \in N-1} F_{\mathrm{T}n,\mathrm{T}N} C_{c,\mathrm{out}}^{\mathrm{T}n} \le F^{\mathrm{T}N} C_{c,\mathrm{in,max}}^{\mathrm{T}N} \qquad \forall c \in C \tag{69}$$

$$M_{c,\mathrm{in}}^{\mathrm{T}N} = \sum_i F_{i,\mathrm{T}N} C_c^i + \sum_{n \in N-1} F_{\mathrm{T}n,\mathrm{T}N} C_{c,\mathrm{out}}^{\mathrm{T}n} \qquad \forall c \in C \tag{70}$$

$$M_{c,\mathrm{out}}^{\mathrm{T}N} = M_{c,\mathrm{in}}^{\mathrm{T}N} (1 - R_c^{\mathrm{T}N}) \qquad \forall c \in C \tag{71}$$

$$\sum_i F_{i,\mathrm{W}} C_c^i + \sum_{n \in N-1} F_{\mathrm{T}n,\mathrm{W}} C_{c,\mathrm{out}}^{\mathrm{T}n} + M_{c,\mathrm{out}}^{\mathrm{T}N} \le C_c^{\mathrm{env}} \left[\sum_i F^i \right] \qquad \forall c \in C \tag{72}$$

$$Mz^{i\,\mathrm{T}N} \le F_{i,\mathrm{T}N} \le F^i z^{i\,\mathrm{T}N} \tag{73}$$

$$Mz^{i\mathrm{W}} \le F_{i,\mathrm{W}} \le F^i z^{i\mathrm{W}} \tag{74}$$

$$Mz^{\mathrm{T}n\mathrm{T}N} \le F_{\mathrm{T}n,\mathrm{T}N} \le F^{\mathrm{T}n} z^{\mathrm{T}n\mathrm{T}N} \qquad \forall n \in N-1 \tag{75}$$

$$Mz^{\mathrm{T}nW} \le F_{\mathrm{T}n,\mathrm{W}} \le F^{\mathrm{T}n} z^{\mathrm{T}nW} \qquad \forall n \in N-1 \tag{76}$$

$$\sum_i z^{i\mathrm{T}N} = A^{\mathrm{T}N} \tag{77}$$

The objective function is to minimize the flowrate treated. At this point, mathematical formulations for the first sequence have been done. This procedure is repeated for the remaining sequences of treatment units.

Parametric Optimization Step. Having explored all possible structures for each BNS that meet the environmental discharge limit, one can then develop superstructures involving all wastewater streams and units, and the discharge point are constructed as shown in Figure 7. In this step, the structures determined by MILP are fixed, and each of these selected structures is optimized for its parametric values using NLP. The mathematical formulations are constructed as follows:

$$F_i = \sum_N F_{i,\mathrm{T}n} + F_{i,\mathrm{W}} \qquad \forall i \in I \tag{78}$$

$$F_{\mathrm{T}n} = \sum_i F_{i,\mathrm{T}n} + \sum_N F_{\mathrm{T}n,\mathrm{T}n} \qquad \forall n \in N \tag{79}$$

$$\sum_i F_{i,\mathrm{T}n} C_c^i + \sum_N F_{\mathrm{T}n,\mathrm{T}n} C_{c,\mathrm{out}}^{\mathrm{T}n} \le F^{\mathrm{T}n} C_{c,\mathrm{in,max}}^{\mathrm{T}n} \qquad \forall c \in C, n \in N \tag{80}$$

$$F_{\mathrm{T}n} C_{c,\mathrm{in}}^{\mathrm{T}n} = \sum_i F_{i,\mathrm{T}n} C_c^i + \sum_N F_{\mathrm{T}n,\mathrm{T}n} C_{c,\mathrm{out}}^{\mathrm{T}n} \qquad \forall c \in C, n \in N \tag{81}$$

$$C_{c,\mathrm{out}}^{\mathrm{T}n} = C_{c,\mathrm{in}}^{\mathrm{T}n} (1 - R_c^{\mathrm{T}n}) \qquad \forall c \in C, n \in N \tag{82}$$

$$F_{\mathrm{T}n} = \sum_N F_{\mathrm{T}n,\mathrm{T}n} + F_{\mathrm{T}n,\mathrm{W}} \qquad \forall n \in N \tag{83}$$

$$\sum_i F_{i,\mathrm{W}} C_c^i + \sum_N F_{\mathrm{T}n,\mathrm{W}} C_{c,\mathrm{out}}^{\mathrm{T}n} \le \left[\sum_i F_{i,\mathrm{W}} + \sum_N F_{\mathrm{T}n,\mathrm{W}} \right] C_c^{\mathrm{env}} \qquad \forall c \in C \tag{84}$$

These formulations are optimized to get the minimum total flowrate treated based on structures obtained before. At this point, the total water system has been optimized systematically, and the approach has provided several total water structures simultaneously.

Total Water System Design

Mathematical formulations for the total water system design are then constructed and the obtained water networks are used

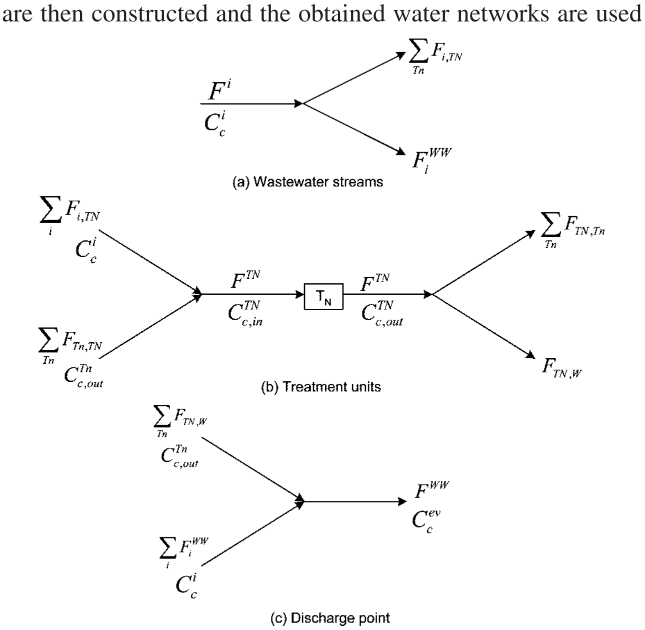

Figure 7. Superstructures of wastewater streams, treatment units, and discharge point.

as the initialization. The formulations are the combined models of NLP formulations for each subsystem (water reuse subsystem, regeneration unit, and wastewater treatment subsystem). In this total system, any water treatment unit (Tn) can be considered as regeneration unit. Initial points from the three subsystems control and direct the NLP optimization solver to produce the solutions that the user wants.

$$F_i^{\mathrm{FW}} + \sum_{I} F_{i',i} + \sum_{J} F_{j,i} + \sum_{N} F_{\mathrm{T}n,i} = F^i \qquad \forall\, i \in I \tag{85}$$

$$F_k^{\mathrm{FW}} + \sum_{I} F_{i,k} + \sum_{J} F_{j,k} + \sum_{N} F_{\mathrm{T}n,k} = F^k \qquad \forall\, k \in K \tag{86}$$

$$F_{\mathrm{FW},i} C_c^{\mathrm{FW}} + \sum_{I} F_{i',i} C_{c,\mathrm{out}}^{i'} + \sum_{J} F_{j,i} C_c^j + \sum_{N} F_{\mathrm{T}n,i} C_{c,\mathrm{out}}^{\mathrm{T}n} = F^i C_{c,\mathrm{in}}^i \le F^i C_{c,\mathrm{in,max}}^i \qquad \forall\, i \in I, c \in C \tag{87}$$

$$F_{\mathrm{FW},k} C_c^{\mathrm{FW}} + \sum_{I} F_{i,k} C_{c,\mathrm{out}}^{i} + \sum_{J} F_{j,k} C_c^j + \sum_{N} F_{\mathrm{T}n,k} C_{c,\mathrm{out}}^{\mathrm{T}n} = F^k C_{c,\mathrm{in}}^k \le F^k C_{c,\mathrm{in,max}}^k \qquad \forall\, k \in K, c \in C \tag{88}$$

$$F^i (C_{c,\mathrm{out}}^i - C_{c,\mathrm{in}}^i) = \Delta m_c^i \qquad \forall\, c \in C, i \in I \tag{89}$$

$$F^i = \sum_{I} F_{i,i'} + \sum_{K} F_{i,k} + \sum_{N} F_{i,\mathrm{T}n} + F_i^{\mathrm{WW}} \qquad \forall\, i \in I \tag{90}$$

$$F^j = \sum_{I} F_{j,i} + \sum_{K} F_{j,k} + \sum_{N} F_{j,\mathrm{T}n} + F_j^{\mathrm{WW}} \qquad \forall\, j \in J \tag{91}$$

$$\sum_{I} F_{i,\mathrm{T}n} + \sum_{J} F_{j,\mathrm{T}n} + \sum_{N} F_{\mathrm{T}n,\mathrm{T}n} = F^{\mathrm{T}n} \qquad \forall\, \mathrm{T}n \in N \tag{92}$$

$$\sum_{I} F_{i,\mathrm{T}n} C_{c,\mathrm{out}}^{i} + \sum_{J} F_{j,\mathrm{T}n} C_c^j + \sum_{N} F_{\mathrm{T}n,\mathrm{T}n} C_{c,\mathrm{out}}^{\mathrm{T}n} = F^{\mathrm{T}n} C_{c,\mathrm{in}}^{\mathrm{T}n} \le F^{\mathrm{T}n} C_{c,\mathrm{in,max}}^{\mathrm{T}n} \qquad \forall\, \mathrm{T}n \in N \tag{93}$$

$$C_{c,\mathrm{out}}^{\mathrm{T}n} = C_{c,\mathrm{in}}^{\mathrm{T}n} (1 - R_c^{\mathrm{T}n}) \qquad \forall\, c \in C, \mathrm{T}n \in N \tag{94}$$

$$F^{\mathrm{T}n} = \sum_{I} F_{\mathrm{T}n,i} + \sum_{K} F_{\mathrm{T}n,k} + \sum_{N} F_{\mathrm{T}n,\mathrm{T}n} + F_{\mathrm{T}n,\mathrm{W}} \qquad \forall\, \mathrm{T}n \in N \tag{95}$$

$$\sum_{I} F_i^{\mathrm{WW}} C_{c,\mathrm{out}}^i + \sum_{J} F_j^{\mathrm{WW}} C_c^j + \sum_{N} F_{\mathrm{T}n,\mathrm{W}} C_{c,\mathrm{out}}^{\mathrm{T}n} \le \left(\sum_{I} F_{i,\mathrm{W}} + \sum_{N} F_{\mathrm{T}n,\mathrm{W}} \right) C_c^{\mathrm{env}} \qquad \forall\, c \in C \tag{96}$$

The objective function for the mathematical expressions of total water system design is to minimize the total freshwater consumption or total annual cost for the total water system.

Case Study

A case study of a total water system design is adapted from the works of Kuo,[8] Alva-Argáez,[9] and Gunaratnam.[12] Tables 1, 2, and 3 show the data of water-using operations, contaminant removal ratio, and the environmental concentration for the total water system, respectively. Cost parameters are presented in Table 4 for both the capital and the operating cost of the treatment units. In this case, the capital and operating cost of the treatment units is proportional to the flowrate of wastewater treated (F). The cost for freshwater supply is \$0.2/t. The plant is assumed to be operating for 8600 h per year with annualization factor of 0.1.

The objective of the case study is to find the cost-effective design of a total water system. Several researchers have solved this problem by using their own methods such as the grouping and migrating approach[8] and an iterative procedure for solving MINLP formulations.[9,12,13]

The proposed two-step optimization approach is demonstrated in this case study. The total water system is decomposed into two subsystems, water-using and wastewater treatment. Each of these subsystems has its own two-step optimization approach. These subsystems are optimized systematically where each of their final solutions will become the basis for the next subsystem. To further reduce freshwater consumption, H_2S steam stripping can be considered as the regeneration unit.[8] This consideration was incorporated as part of the automated and iterative optimization of MINLP formulations.[9,12,13] Following the aforementioned procedure and taking the treatment unit T1 (H_2S steam stripping), several total water networks are generated as a "family of good solutions" for design comparison (from Figures 8–11).

The two total water system structures above consume and discharge 58 t/h of freshwater and wastewater, respectively. The two structures highlight three direct water reuse streams, one regeneration−reuse stream, and one regeneration−recycling stream. The direct water reuse streams are WUO1-WUO2, WUO1-WUO5, and WUO4-WUO2. The regeneration-reuse stream is shown by T1-WUO3, and the regeneration-recycling stream is T1-WUO2-T1.

The difference between them is in the sequence of wastewater treatment units. As in reality, the placement of API oil/water

Table 1. Water-Using Operations for the Total Water System

process	contaminant	mass load (g/hr)	$C_{\max,\mathrm{in}}$ (ppm)	$C_{\max,\mathrm{out}}$ (ppm)	F_{lim} (t/h)
WUO1	HC	750	0	15	50
	H_2S	20000	0	400	50
	SS	1750	0	35	50
WUO2	HC	3400	20	120	34
	H_2S	414800	300	12500	34
	SS	4590	45	180	34
WUO3	HC	5600	120	220	56
	H_2S	1400	20	45	56
	SS	520800	200	9500	56
WUO4	HC	160	0	20	8
	H_2S	480	0	60	8
	SS	160	0	20	8
WUO5	HC	800	50	150	8
	H_2S	60800	400	8000	8
	SS	480	60	120	8

Table 2. Contaminant Removal Ratio for Each Treatment Unit

operation	removal ratio		
	HC	H_2S	SS
T1 (H_2S steam stripping)	0	0.999	0
T2 (biological treatment unit)	0.7	0.9	0.98
T3 (API oil/water separator)	0.95	0	0.5

Table 3. Environmental Concentration Limits for Each Contaminant

component	concentration (ppm)
HC	20
H_2S	5
SS	100

Table 4. Cost Parameters for Treatment Units[a]

cost parameters	steam-stripping column (T1)	biological treatment unit (T2)	API oil/water separator (T3)
capital cost (\$)	$16800F^{0.7}$	$12600F^{0.7}$	$4800F^{0.7}$
operating cost (\$/h)	$1F$	$0.0067F$	0

[a] Note: F = wastewater flowrate treated in the respective treatment unit.

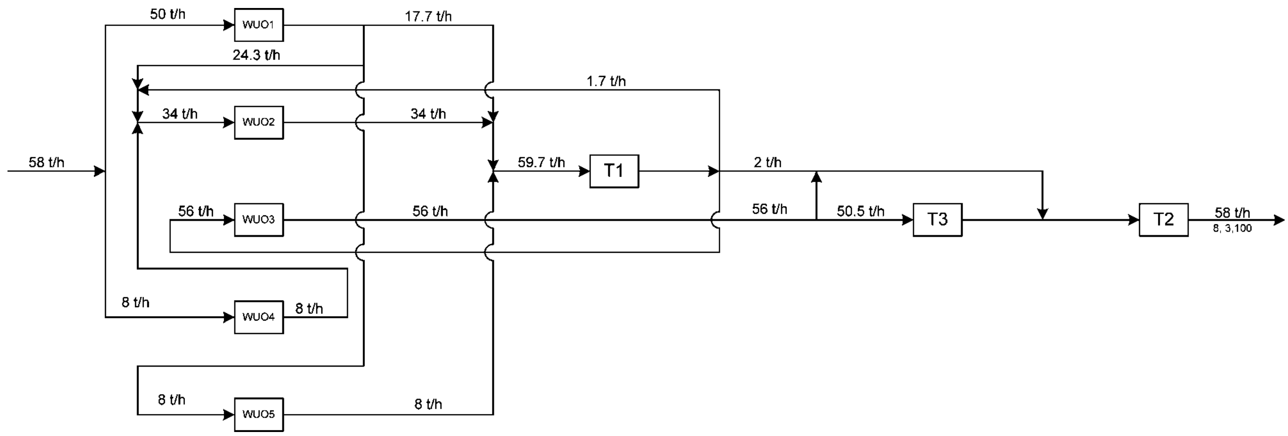

Figure 8. Total water system design (Structure 1) generated by the proposed method.

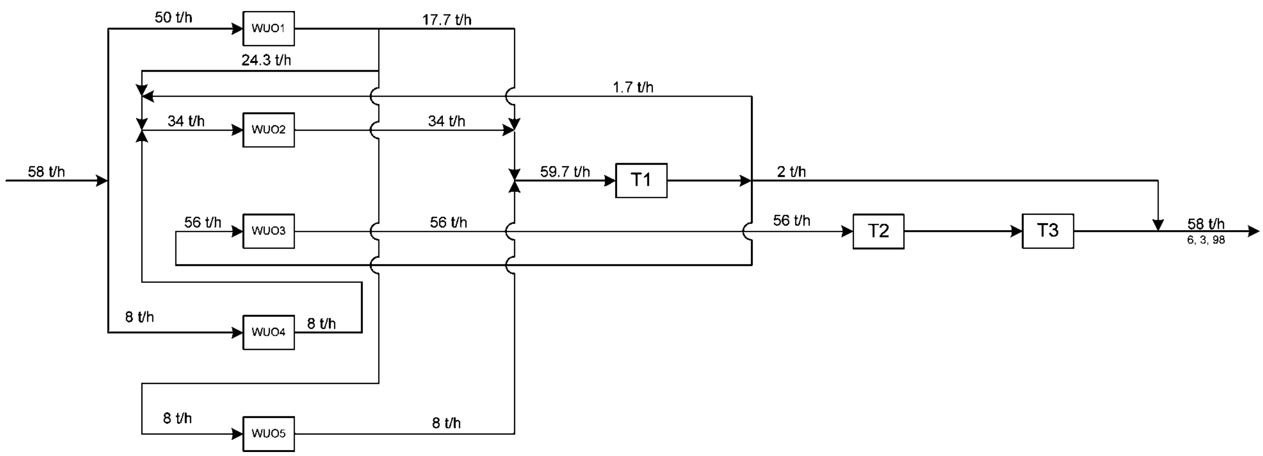

Figure 9. Alternative total water system design using the proposed approach.

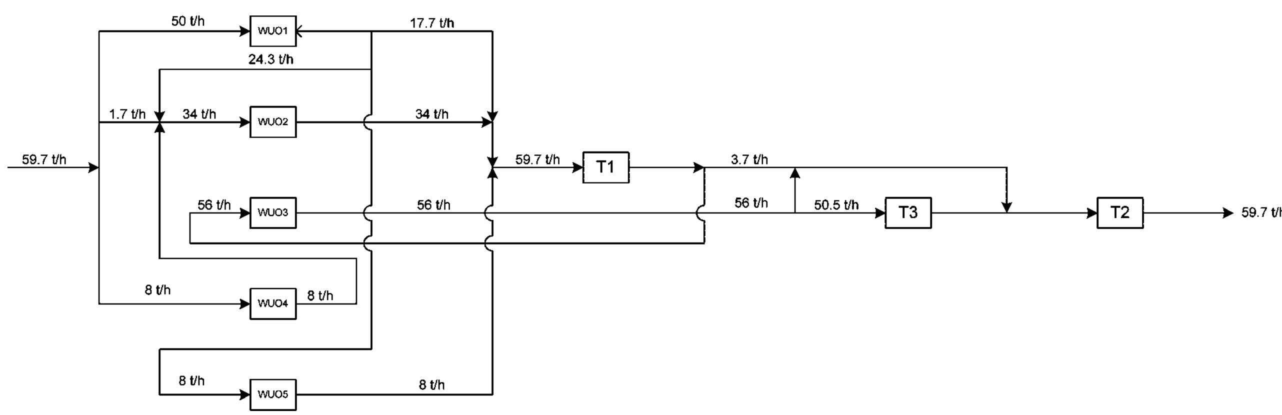

Figure 10. Modification of Structure 1 without regeneration-recycling loop (Structure 2).

separator (T3) should be in the upstream of the biological treatment unit (T2). The performance of the API oil/water separator is higher when it receives higher inlet contaminant, and in any case, oil waste should be separated from the wastewater before handling the waste in the biological treatment.[18] This insight was not captured by the automated optimization of MINLP as developed by the previous researchers[9,12,13] because they did not consider this practical issue in the first place. It can be argued that by controlling their MINLP formulations, they may get a similar water network design. However, this argument has not been demonstrated in their work as their approach is aimed at generating a single optimum solution without allowing user interaction during the optimization process. In this case, Figure 9 can then be removed from the list of solutions.

Structure 1 has a regeneration recycling loop from H2S steam stripping (T1) to water-using operation 2 (WUO2). Considering regeneration recycling is not allowed due to the possibility of accumulation of certain contaminants in the water-using operations, the option in Figure 10 can be proposed.

Figure 10 shows the modification of Structure 1 as a result from the two-step optimization approach where the regeneration−recycling loop is not allowed. The modified structure has only three direct water-reused streams and one regeneration−reused stream. The total water system consumes slightly higher freshwater than before, which is 59.7 t/hr. Figure 11

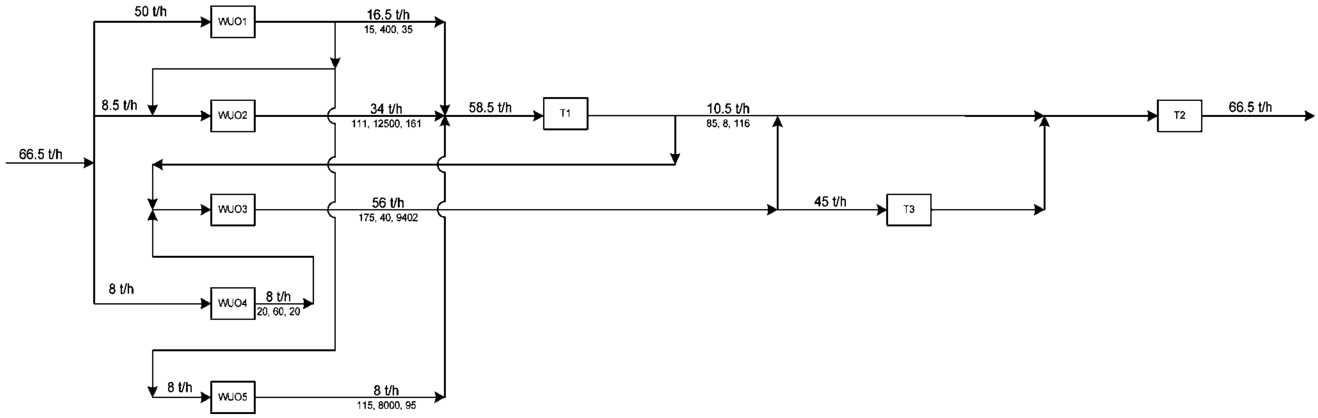

Figure 11. Total water system design (Structure 3) option shows relatively simple pipework.

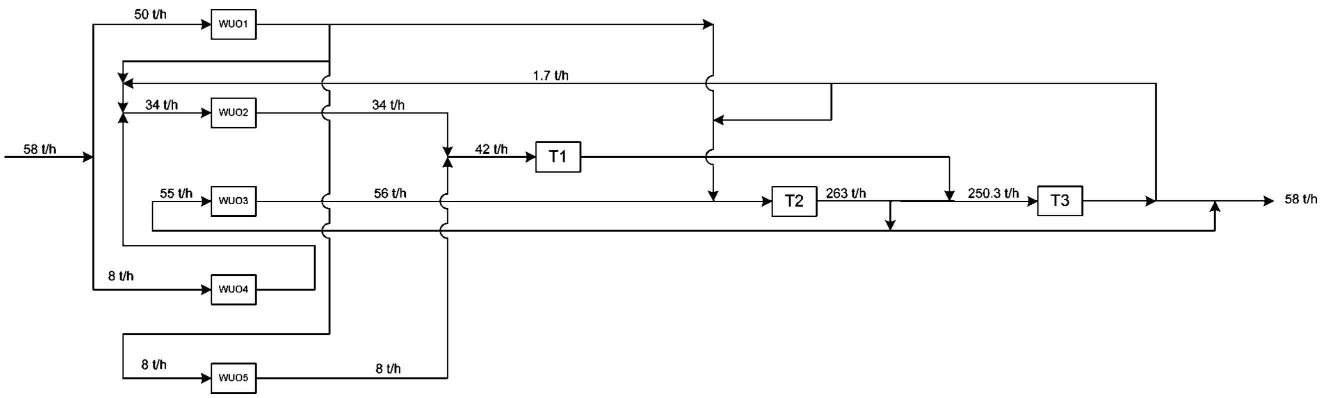

Figure 12. Total water system obtained by automated optimization of MINLP,[9,12,13] allowing regeneration-recycling loop.

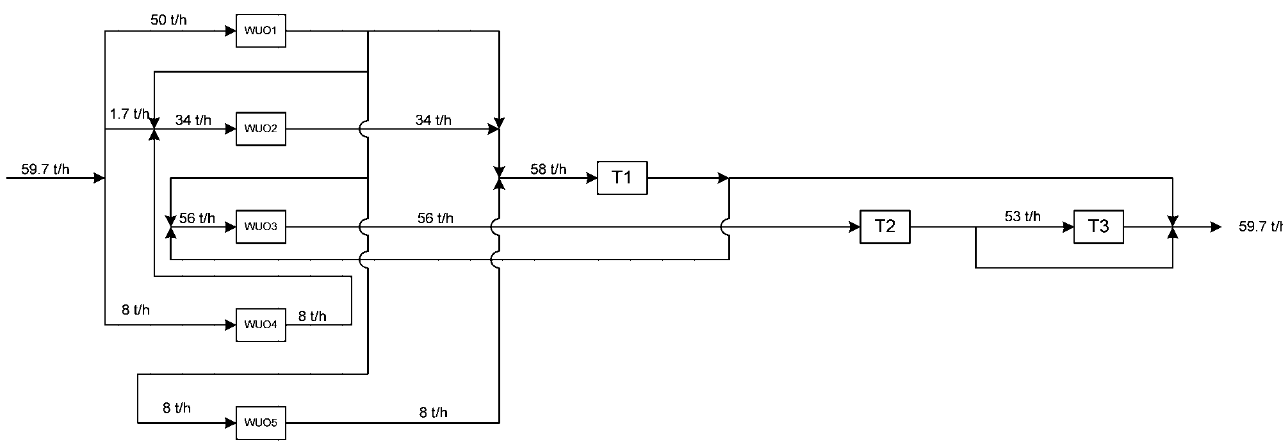

Figure 13. Total water system design by automated optimization of MINLP;[9,12,13] regeneration-recycling is not allowed.

below shows another total water system with higher freshwater consumption, 66.5 t/h. This structure also shows three direct water reused streams and one regeneration-reused stream. The direct water reuse streams are WUO1-WUO2, WUO1-WUO5, and WUO4-WUO3. The regeneration-reused stream is T1-WUO3.

The optimum solution obtained by automated optimization of MINLP[9,12,13] is shown in Figure 12 where the regeneration-recycling loop is allowed. It shows three direct water reused streams and two regeneration-recycling streams. This solution features more complicated wastewater treatment piping interconnections. Figure 13 is the optimum solution where regeneration-recycling is not allowed. Thus, it gives simpler water system design than the one in Figure 12. However, it has more water reuse streams than the solution given by the two-step optimization approach here. It has four direct water reused streams, namely, WUO1-WUO2, WUO1-WUO3, WUO1-WUO5, and WUO4-WUO2. It also has one regeneration-reused stream, T1-WUO3. Nonetheless, the two optimum solutions as reported by the automated optimization of MINLP[9,12,13] have limitations on the practicality of the placement of the biological treatment unit in the upstream of the API oil/water separator. This kind of placement appears from the automated programming whose objective function is to minimize the total cost. Even though common practical considerations have been considered, such process constraints can be missed out during the optimization process.

Total water system designed by operation migration and a grouping approach,[8] as shown in Figure 14, produces a more practical design where the API oil/water separator is placed on

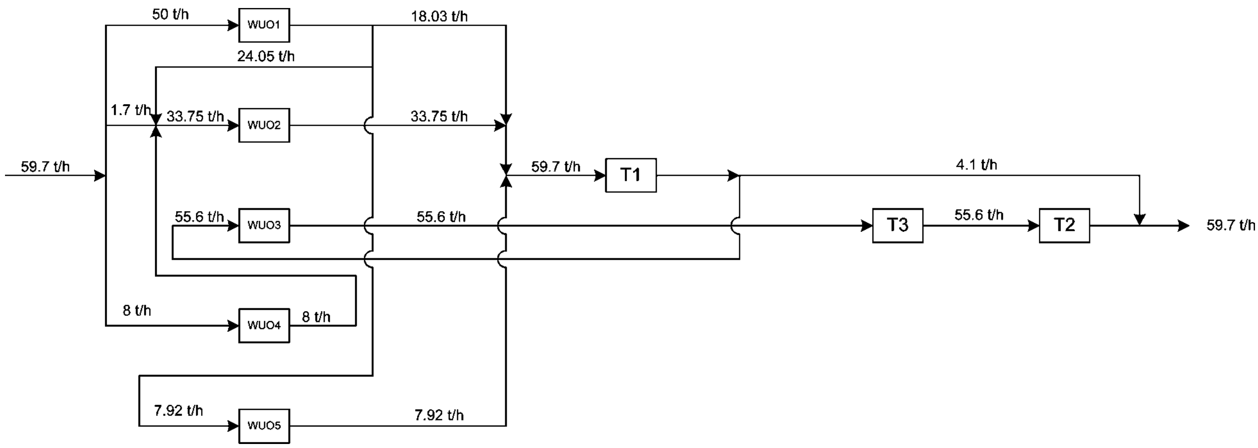

Figure 14. Total water system design obtained from the work of Kuo.[8]

Table 5. Economic Comparison for Total Water System Designs

cost calculation ($/year)	Figure 8	Figure 9	Figure 10	Figure 11	Figure 12	Figure 13	Figure 14
freshwater supply	99 760	99 760	102 684	114 380	99 760	102 684	102 684
capital treatment cost	590 603	590 603	589 409	608 168	1 081 884	576 433	583 900
operating treatment cost	516 762	516 762	516 860	506 932	376 354	502 027	516 624
total cost ($/year)	675 582	675 582	678 485	682 129	584 303	662 354	677 698

the upstream of the combined biological treatment unit. However, this solution is obtained graphically, which is very cumbersome when applied in a complex problem.

Table 5 shows the economic calculation for all of the total water system designs resulted from the two-step optimization approach and the previous works. The calculation procedure is adopted from others[4] by using the presented economic data in Table 4 and the cost of the freshwater supply. The total water system design in Figure 12, which is obtained from the automated optimization of MINLP,[9] results in the lowest total annual cost with $584 303/year. The design has the lowest operating treatment cost even though it has the most complex piping configuration and the biggest design of the biological treatment unit and API oil/water separator. Figure 11 shows a design that contributes to the highest total annual cost of $682 129/year because it consumes a higher freshwater supply. The rest of the designs provide comparable results with respect to the total annual cost.

Conclusion

The two-step optimization approach has been presented as an alternative solution strategy for total water system design problem. The approach has been used to solve a case study taken from the literature. The solutions obtained show comparable results in terms of total annual cost, freshwater savings, wastewater discharge, and piping complexity of the structures. The approach proves to be a user interactive tool when considering process and practical constraints. It can also produce multiple solutions toward a minimum target of freshwater consumption and/or total annual cost. Users can assess these solutions and select the one that meets their requirements.

Acknowledgment

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Nomenclature

Δm_c^i = mass load of contaminant c picked up in operation unit i, (kg/h)
A = number of wastewater streams mixed at the inlet of treatment unit n (Tn)
C_c^{FW} = concentration of contaminant c in freshwater (ppm)
$C_{c,\mathrm{in}}^i$ = inlet concentration of contaminant c for operation i (ppm)
$C_{c,\mathrm{in,max}}^i$ = maximum inlet concentration of contaminant c for operation i (ppm)
$C_{c,\mathrm{out}}^i$ = outlet concentration of contaminant c for operation i (ppm)
$C_{c,\mathrm{out,max}}^i$ = Maximum outlet concentration of contaminant c for operation i (ppm)
C_c^j = concentration of contaminant c in source stream j (ppm)
C_c^k = concentration of contaminant c in sink stream k (ppm)
$C_{c,\mathrm{in}}^{\mathrm{regen}}$ = inlet concentration of contaminant c for the regeneration unit (ppm)
$C_{c,\mathrm{out}}^{\mathrm{regen}}$ = outlet concentration of contaminant c for the regeneration unit (ppm)
$C_{c,\mathrm{in}}^{\mathrm{T1}}$ = inlet concentration of contaminant c for treatment unit T1 (ppm)
$C_{c,\mathrm{out}}^{\mathrm{T1}}$ = outlet concentration of contaminant c for treatment unit T1 (ppm)
$C_{c,\mathrm{in,max}}^{\mathrm{T1}}$ = maximum allowable inlet concentration of contaminant c for treatment unit T1 (ppm)
$C_{c,\mathrm{in,max}}^{\mathrm{T2}}$ = maximum allowable inlet concentration of contaminant c for treatment unit T2 (ppm)
$C_{c,\mathrm{in,max}}^{\mathrm{T}N}$ = maximum allowable inlet concentration of contaminant c for the considered treatment unit N (TN) (ppm)
$C_{c,\mathrm{in}}^{\mathrm{T}n}$ = inlet concentration of contaminant c for treatment unit n (Tn) (ppm)
$C_{c,\mathrm{out}}^{\mathrm{T}n}$ = outlet concentration of contaminant c for treatment unit n (Tn) (ppm)
C_c^{env} = concentration of contaminant c for discharge to environment (ppm)
$F_{\mathrm{total}}^{\mathrm{FW}}$ = total freshwater consumption (t/h)
F_i^{FW} = freshwater flowrate to operation i (t/h)
F_k^{FW} = freshwater flowrate to sink k (t/h)
F^i = water flowrate through operation i (t/h)
$F_{i,i'}$ = water reused flowrate from operation i to operation i' (t/h)

$F_{i,k}$ = water reused flowrate from operation i to sink k (t/h)
F_i^{WW} = water flowrate from operation i to discharge (t/h)
$F_{i',i}$ = water reused flowrate from operation i' to operation i (t/h)
F^j = water flowrate from source j (t/h)
$F_{j,i}$ = water reused flowrate from operation j to operation i (t/h)
$F_{j,k}$ = water reused flowrate from source j to sink k (t/h)
F_j^{WW} = water flowrate from source j to discharge (t/h)
F^k = water flowrate to sink k (t/h)
$F_{i,r}$ = water flowrate from operation i to regeneration unit r (t/h)
F_{regen} = water flowrate through regeneration unit r (t/h)
$F_{r,k}$ = water flowrate from regeneration unit r to sink k (t/h)
$F_{j,r}$ = water flowrate from source j to regeneration unit r (t/h)
F_r^{WW} = water flowrate from regeneration unit r to discharge (t/h)
$F_{i,T1}$ = wastewater flowrate from stream i to treatment unit T1 (t/h)
$F_{i,T2}$ = wastewater flowrate from stream i to treatment unit T2 (t/h)
F^{T1} = wastewater flowrate through treatment unit T1 (t/h)
F^{T2} = wastewater flowrate through treatment unit T2 (t/h)
$F_{T1,T2}$ = wastewater flowrate from treatment unit T1 to treatment unit T2 (t/h)
F_{iT3} = wastewater flowrate from stream i to treatment unit T3 (t/h)
$F_{T1,T3}$ = wastewater flowrate from treatment unit T1 to treatment unit T3 (t/h)
$F_{T1,W}$ = wastewater flowrate from treatment unit T1 to discharge (t/h)
$F_{i,TN}$ = wastewater flowrate from stream i to the considered treatment unit N (TN) (t/h)
$F_{i,W}$ = wastewater flowrate from stream i to discharge (t/h)
F^{Tn} = wastewater flowrate through treatment unit n (Tn) (t/h)
$F_{Tn,TN}$ = wastewater flowrate from treatment unit n (Tn) to treatment unit N (TN), where n is any treatment unit preceding the considered treatment unit N (t/h)
$F_{Tn,W}$ = wastewater flowrate from treatment unit n (Tn) to discharge (t/h)
F^{TN} = wastewater flowrate through the considered treatment unit N (TN) (t/h)
$L_{c,in}^{regen}$ = inlet mass load of contaminant c for regeneration unit (kg/h)
$L_{c,out}^{regen}$ = outlet mass load of contaminant c for regeneration unit (kg/h)
M = minimum water flowrate permitted to flow through pipes
$M_{c,in}^{T1}$ = inlet mass load of contaminant c for treatment unit T1 (kg/h)
$M_{c,out}^{T1}$ = outlet mass load of contaminant c for treatment unit T1 (kg/h)
$M_{c,in}^{T2}$ = inlet mass load of contaminant c for treatment unit T2 (kg/h)
$M_{c,out}^{T2}$ = outlet mass load of contaminant c for treatment unit T2 (kg/h)
$M_{c,in}^{TN}$ = inlet mass load of contaminant c for treatment unit N (TN) (kg/h)
$M_{c,out}^{TN}$ = outlet mass load of contaminant c for treatment unit N (TN) (kg/h)
N = level of piping complexity (total number of reused streams)
P = maximum number of reused streams attached to operation i
Q = maximum number of reused streams attached to sink k
R_c^{regen} = removal ratio for contaminant c in regeneration unit
R_c^{T1} = removal ratio for contaminant c in treatment unit T1
R_c^{T2} = removal ratio for contaminant c in treatment unit T2
R_c^{TN} = removal ratio for contaminant c in the considered treatment unit N (TN)
R_c^{Tn} = removal ratio for contaminant c in treatment unit n (Tn)
W = water flowrate discharged to the environment (t/h)

$z^{ii'}$ = binary variables for reused stream from operation i to operation i'
z^{ik} = binary variables for reused stream from operation i to sink k
z^{ji} = binary variables for reused stream from source j to operation i
z^{jk} = binary variables for reused stream from source j to sink k
z^{rk} = Binary variables for regenerated water from regeneration unit r to sink k
z^{iT1} = binary variables for wastewater stream from stream i to treatment unit T1
z^{iT2} = binary variables for wastewater stream from stream i to treatment unit T2
z^{iW} = binary variables for wastewater stream from stream i to discharge
z^{iT3} = binary variables for wastewater from stream i to treatment unit T3
z^{T1T2} = binary variables for wastewater from treatment unit T1 to treatment unit T2
z^{T1T3} = binary variables for wastewater from treatment unit T1 to treatment unit T3
z^{T1W} = binary variables for wastewater from treatment unit T1 to discharge
z^{T2W} = binary variables for wastewater from treatment unit T2 to discharge
z^{iTN} = binary variables for wastewater from stream i to the considered treatment unit N (TN)
z^{TnTN} = binary variables for wastewater from treatment unit n (Tn) to the considered treatment unit N (TN)
z^{TnW} = binary variables for wastewater from treatment unit n (Tn) to discharge

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