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Development of a Generalized Mixed Integer Nonlinear Programming Model for Assessing and Improving the Operational Flexibility of Water Network Designs

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In designing and operating any water network, a typical issue that must be addressed is concerned with the uncertain process conditions. A systematic procedure is proposed in this paper to enhance the operational flexibility of a given structure. Specifically, two design options have been investigated: (1) relaxation of the allowed maximum freshwater consumption rate in the nominal design and (2) installation of auxiliary pipelines and/or elimination of existing ones. The flexibility index model proposed by Swaney and Grossmann (1985) has been modified and formulated in a generalized format to evaluate the impact of introducing various modifications into an existing network. Since this model is a mixed integer nonlinear program (MINLP), it is in general very difficult to locate the global optima in the iterative solution processes. A simple and effective initialization procedure has also been devised in this work to facilitate successful convergence. The effectiveness of the proposed approach is demonstrated with two examples in this paper.

Introduction

In recent years, the important issues of freshwater conservation and wastewater reduction have drawn increasing attention in the process industries.[1] Process integration techniques have often been adopted to realize the reuse, regeneration−reuse, and regeneration−recycling of process and utility waters in chemical plants.[2−4] In implementing these design procedures, it is usually assumed that the process data are fixed and well-defined. However, the actual operating conditions of the freshwater supplier and the basic processing units in a water network, for example, the mass loads of water users, the removal ratios of treatment operations, and the upper limits of contaminant concentrations at the inlet and outlet of each unit, may fluctuate over time. Such fluctuations could lead to deterioration in the water qualities of effluents and even operation disruption if the water network design is not flexible enough to cope with these uncertain disturbances.[5,6]

In general, the term "flexibility" is considered as the capability of a process to function adequately over a given range of uncertain conditions.[7,8] There are in fact very few reported studies devoted specifically to the design problems of resilient water networks. Tan and Cruz[9] built two linear models for the synthesis of robust water-reuse networks from imprecise data using the symmetry fuzzy linear programming (SFLP) method. It was assumed that the sources of uncertainties stemmed from disturbances in mass loads and also in upper limits of inlet concentrations. Al-Redhwan, Crittenden, and Lababidi[10] developed a three-step procedure to design water networks under uncertain operating temperatures and pressures. Karuppiah and Grossmann[5] studied a similar problem, and proposed a spatial branch-and-cut algorithm to locate the global optimum. Tan, Foo, and Manan[6] used the Monte Carlo simulation techniques to access the vulnerability of water networks which are subject to noisy mass loads. Zhang, Feng, and Qian[2] suggested to use the concept of maximum tolerance amount of a water unit (MToAWU), rank of unit (RU) and outflow branch number of unit (OBNU) to quantify the resiliency of a given water network.

It is generally recognized that the aforementioned design strategies are still not mature enough for generating cost-optimal water networks which are also resilient under the influences of uncertain disturbances.[2] There is thus a need to develop systematic techniques to improve the operational flexibility of one or more given network obtained on the basis of economic criteria only. To this end, two design options have been thoroughly studied in the present work, that is, (1) relaxation of the upper limit of freshwater supply rate and (2) installation of auxiliary pipelines and/or elimination of original ones. The flexibility index model proposed by Swaney and Grossmann[11] has been modified and formulated in a generalized format to evaluate the impacts of introducing various combinations of these additional features into an existing network. The uncertain disturbances considered are those in the freshwater quality, the mass loads of water-using units, the removal ratios of wastewater treatment units, and the maximum inlet and outlet concentrations of these two types of units. The control variables used for compensating disturbances are assumed to be the freshwater consumption rate and the flow ratios associated with the outward branches connected to every splitter in the network. Since the flexibility index model is a complex mixed integer nonlinear program (MINLP), the global optimum cannot always be obtained in the iterative solution process. A good initial guess is often needed to facilitate the search process. To satisfy this need, a simple and effective initialization procedure[12] has also been developed in this work to systematically solve the MINLP models within GAMS environment.[13]

The remaining paper is organized as follows. A concise problem statement is first provided in the next section. Next the detailed formulation of the generalized flexibility index model is given in section 3. The implementation procedures for incorporating the aforementioned design options in a given network are then presented in section 4. To demonstrate the effectiveness of the proposed approach, the numerical results

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obtained in two case studies are described in section 5. Finally, conclusions and future works are outlined in the last section.

Problem Statement

As mentioned previously, the primary objective of this work is to develop a set of systematic methods to assess and then enhance the operational resiliency of one or more given nominal water-network designs. A nominal design should include specifications of the freshwater consumption rate, the effluent flow rates, all unit throughputs, the network configuration, the water flow rate in every branch, and the contaminant concentrations at the sinks and the inlets and outlets of all water-using and wastewater-treatment units.

The flexibility index model developed by Swaney and Grossmann[11] has been adopted to determine a quantitative measure for use as the selection criterion of additional features to be introduced into the nominal design. Its model structure is outlined below to facilitate a clear presentation of the problem statement. Specifically, the equality and inequality constraints of this optimization problem can be expressed in a general form as

$$\mathbf{h}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) = 0 \tag{1}$$

$$\mathbf{g}(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) \leq 0 \tag{2}$$

where $\mathbf{h} = 0$ denotes a system of equations which are used in this model to characterize mass balances and also unit performances and $\mathbf{g} \leq 0$ represents the inequalities used to stipulate the design specifications and physical constraints which must be enforced to ensure feasible operation. In the above constraints, $\mathbf{d}$ is a vector of design parameters which define the network structure and equipment sizes. Their values are determined at the design stage and should be treated as constants during plant operation. In particular, these fixed design parameters include the maximum freshwater supply rate, the maximum throughputs of all water-using and wastewater-treatment units, and the upper bounds of pollutant concentrations in effluents. The other process variables can be classified into two groups, that is, the control variables in vector $\mathbf{z}$ and the state variables in vector $\mathbf{x}$. Finally, θ is the vector of uncertain parameters. Notice that dim $\mathbf{x}$ = dim $\mathbf{h}$. Thus, the vector size of $\mathbf{z}$ can be considered as the degree of freedom that is available during plant operation. In other words, the control variables can be adjusted for different realizations of the uncertain parameters θ during operation. Two alternative sets of control variables can be chosen for a given water network: (1) the flow rates of all connecting branches and (2) the freshwater consumption rates and the split ratios associated with the outward branches of every splitter.

Generally speaking, the flexibility level in a given process is dependent upon the maximum range of variation in each uncertain parameter that the plant can tolerate. The so-called flexibility index δ (≥ 0) is a measure of the largest size of feasible operation region in the space of θ. More specifically, this parameter space Θ can be expressed as

$$\Theta(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\} \tag{3}$$

where, θ^N is a vector of parameter values from which the nominal water-network design is obtained, and $\Delta\theta^+$ and $\Delta\theta^-$ denote the expected deviations of uncertain parameters from their nominal values in the positive and negative directions respectively. In this study, the uncertain parameters are assumed to be the freshwater quality, the mass loads of water-using units, the removal ratios of wastewater-treatment units, and the maximum inlet and outlet concentrations of these two types of units. It is also assumed that these parameters can vary *independently* within their specified intervals.

It is our intention to answer the following two important questions with the aforementioned flexibility index model: (1) Is the given nominal design flexible enough? (2) If not, can it be improved by relaxing the upper limit of freshwater supply rate and/or by modifying the network structure of the given design?

Generalized Flexibility Index Model

Since it is very tedious and inefficient to construct different versions of the flexibility index model for various candidate network configurations and then carry out the needed optimization computations, a generalized model has been formulated and used in this work as a design tool for all possible alternative structures.

Superstructure. To develop the general model, it is necessary to first build a superstructure in which all possible flow connections are embedded. The superstructure presented here is essentially a modified version of that suggested by Chang and Li.[4] In its original form, a distinct label is assigned to each of the given water-using units, wastewater-treatment units, water source and sink, that is,

$$\mathbb{U} = \{u \mid u \text{ is the label of a water-using unit in the plant}\} \tag{4}$$

$$\mathbb{T} = \{t \mid t \text{ is the label of a water-treatment unit in the plant}\} \tag{5}$$

$$\mathbb{W} = \{w \mid w \text{ is the label of a water source}\} \tag{6}$$

$$\mathbb{D} = \{d \mid d \text{ is the label of a water sink}\} \tag{7}$$

Notice that the water sources in set $\mathbb{W}$ can be further classified into two subsets: $\mathbb{W} = \mathbb{W}_1 \cup \mathbb{W}_2$, and

$$\mathbb{W}_1 = \{w_1 \mid w_1 \text{ is the label of a freshwater source}\} \tag{8}$$

$$\mathbb{W}_2 = \{w_2 \mid w_2 \text{ is the label of a secondary source}\} \tag{9}$$

In the superstructure used in our study, a set of extra "mixers" are incorporated for the purpose of providing additional configurational options that could be consider in the network design, that is,

$$\mathbb{A} = \{a \mid a \text{ is the label of a fictitious mixer unit}\} \tag{10}$$

where the total number of mixers is a designer-selected parameter.

On the basis of the above definitions, the superstructure construction procedure can be outlined below:

(1) Place a mixing node at the inlet of every water-using unit in $\mathbb{U}$, every wastewater-treatment unit in $\mathbb{T}$, every sink in $\mathbb{D}$, and every mixer in $\mathbb{A}$.

(2) Place a splitting node after every freshwater source in $\mathbb{W}_1$. The split branches from this node are connected to all mixing nodes before the water users in $\mathbb{U}$, the sinks in $\mathbb{D}$, and the mixers in $\mathbb{A}$.

(3) Place a splitting node after every secondary water source in $\mathbb{W}_2$, every water-using unit in $\mathbb{U}$, every wastewater-treatment unit in $\mathbb{T}$, and every mixer in $\mathbb{A}$. The split branches from each node are connected to all the mixing nodes established in step 1.

This scheme can be represented by Figure 1, in which the symbols S and M denote the splitting and mixing node, respectively.

Process Constraints. Let us first introduce the following set definitions to facilitate concise model formulation:

$$\mathbb{P}_1 = \mathbb{U} \cup \mathbb{A} \tag{11}$$

$$\mathbb{P}_2 = \mathbb{U} \cup \mathbb{T} \cup \mathbb{A} \tag{12}$$

$$\mathbb{M} = \mathbb{U} \cup \mathbb{T} \cup \mathbb{D} \tag{13}$$

A set of equality constraints can then be formulated to satisfy process requirements according to Figure 1. These constraints are presented below:

(1) At the splitting nodes originated from primary and secondary water sources, the generalized flow balance equations can be written as

$$\mathrm{sr}_w = \sum_{p \in \mathbb{P}_\ell} f^W_{w,p} + \sum_{d \in \mathbb{D}} f^W_{w,d} \qquad w \in \mathbb{W}_\ell \tag{14}$$

where, $\ell \in \{1, 2\}$; sr_w is the total water supply rate from source w; $f^W_{w,p}$ and $f^W_{w,d}$ denote the flow rates of waters (from source w) which are consumed by processing unit p and sink d, respectively. Since the secondary waters must be completely consumed and their supply rates are assumed to be constants in this study, the following constraints should also be imposed

$$\mathrm{sr}_w = S^{(2)}_w \qquad w \in \mathbb{W}_2 \tag{15}$$

where, $S^{(2)}_w$ is a constant parameter.

(2) The generalized water balance equation at the splitting node from the outlet of a process unit p can be expressed as

$$f^{\mathrm{out}}_p = \sum_{p' \in \mathbb{P}_2} f_{p,p'} + \sum_{d \in \mathbb{D}} f^D_{p,d} \qquad p \in \mathbb{P}_2 \tag{16}$$

where f^{out}_p is the water flow rate at the outlet of unit p; $f_{p,p'}$ represents the water flow rate from unit p to unit p'; $f^D_{p,d}$ is the flow rate of wastewater generated by unit p and sent to sink d.

(3) At the inlet of each processing unit, the water balance around the mixing node can be written as

$$f^{\mathrm{in}}_p = \sum_{p' \in \mathbb{P}_2} f_{p',p} + \sum_{w \in \tilde{\mathbb{W}}} f^W_{w,p} \qquad p \in \mathbb{P}_2 \tag{17}$$

where, f^{in}_p is the total flow rate at the mixing node of unit p; $f_{p',p}$ is the water flow rate from unit p' to unit p; $f^W_{w,p}$ is the water flow rate from source w to unit p and

$$\tilde{\mathbb{W}} = \begin{cases} \mathbb{W}_1 \cup \mathbb{W}_2 & \text{if} \quad p \in \mathbb{U} \cup \mathbb{A} \\ \mathbb{W}_2 & \text{if} \quad p \in \mathbb{T} \end{cases} \tag{18}$$

In this study, the possibility of water loss is not considered in any part of the processing unit. Therefore,

$$f^{\mathrm{in}}_p = f^{\mathrm{out}}_p \qquad p \in \mathbb{P}_2 \tag{19}$$

In addition, the corresponding mass balance of contaminant ξ should be

$$f^{\mathrm{in}}_p c^{\mathrm{in}}_{p,\xi} = \sum_{p' \in \mathbb{P}_2} f_{p',p} c^{\mathrm{out}}_{p',\xi} + \sum_{w \in \tilde{\mathbb{W}}} f^W_{w,p} \bar{C}_{w,\xi} \theta^W_{w,\xi} \qquad p \in \mathbb{P}_2 \qquad \xi \in \mathbb{C} \tag{20}$$

where $\mathbb{C}$ is the set of all contaminants; $c^{\mathrm{in}}_{p,\xi}$ and $c^{\mathrm{out}}_{p',\xi}$ denote the concentrations of contaminant ξ at the inlet of unit p and outlet of unit p' respectively; $\bar{C}_{w,\xi}$ denotes the nominal concentration of contaminant ξ from water source w and $\theta^W_{w,\xi}$ is the corresponding uncertain multiplier.

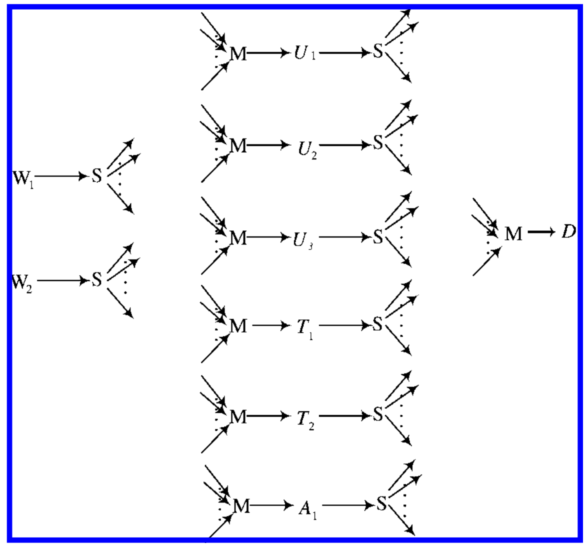

Figure 1. Superstructure of water network.

(4) The process performance of a water-using unit can be characterized as

$$f^{\mathrm{in}}_u c^{\mathrm{in}}_{u,\xi} + \theta^M_{u,\xi} \bar{M}_{u,\xi} = f^{\mathrm{out}}_u c^{\mathrm{out}}_{u,\xi} \qquad u \in \mathbb{U} \qquad \xi \in \mathbb{C} \tag{21}$$

where $c^{\mathrm{in}}_{u,\xi}$ and $c^{\mathrm{out}}_{u,\xi}$, respectively, represent the inlet and outlet concentrations of contaminant ξ of water-using unit u; $\bar{M}_{u,\xi}$ denotes the nominal mass load of contaminant ξ of unit u and $\theta^M_{u,\xi}$ is the corresponding uncertain multiplier.

(5) For each wastewater-treatment unit, the performance equation is

$$c^{\mathrm{out}}_{t,\xi} = c^{\mathrm{in}}_{t,\xi}(1 - \theta^R_{t,\xi} \bar{R}_{t,\xi}) \qquad t \in \mathbb{T} \qquad \xi \in \mathbb{C} \tag{22}$$

where $c^{\mathrm{in}}_{t,\xi}$ and $c^{\mathrm{out}}_{t,\xi}$ represent the inlet and outlet concentrations of contaminant ξ of wastewater-treatment unit t respectively; $\bar{R}_{t,\xi}$ denotes the nominal value of removal ratio of contaminant ξ of unit t and $\theta^R_{t,\xi}$ is the corresponding uncertain multiplier.

(6) For any mixer, the corresponding performance equation can simply be written as

$$c^{\mathrm{in}}_{a,\xi} = c^{\mathrm{out}}_{a,\xi} \qquad a \in \mathbb{A} \qquad \xi \in \mathbb{C} \tag{23}$$

where, $c^{\mathrm{in}}_{a,\xi}$ and $c^{\mathrm{out}}_{a,\xi}$ are the inlet and outlet concentrations of contaminant ξ of mixer a, respectively

(7) At the mixing node of each sink d, the flow and contaminant balances are

$$f^{\mathrm{in}}_d = \sum_{p \in \mathbb{P}_2} f^D_{p,d} + \sum_{w \in \mathbb{W}} f^W_{w,d} \qquad d \in \mathbb{D} \tag{24}$$

$$f^{\mathrm{in}}_d c^{\mathrm{in}}_{d,\xi} = \sum_{p \in \mathbb{P}_2} f^D_{p,d} c^{out}_{p,\xi} + \sum_{w \in \mathbb{W}} f^W_{w,d} \bar{C}_{w,\xi} \theta^W_{w,\xi} \qquad d \in \mathbb{D} \qquad \xi \in \mathbb{C} \tag{25}$$

where, f^D_d is the total water flow rate after the mixing node of sink d; $c^{\mathrm{in}}_{d,\xi}$ is the corresponding concentration of contaminant ξ; $\bar{C}_{w,\xi}$ is the nominal value of the concentration of contaminant ξ at source w and $\theta^W_{w,\xi}$ is the corresponding uncertain multiplier.

To further simplify model formulation, let us introduce a set of unified labels to represent the aforementioned equality constraints, that is,

$$\mathbb{I} = \{i \mid i \text{ is the label of an equality process constraint}\} \tag{26}$$

Thus, all equality constraints can by written in a general form as

$$h_i = 0 \qquad i \in \mathbb{I} \tag{27}$$

It should be noted that, other than the equality constraints, some of the process requirements may be expressed as inequality constraints:

(1) The upper bounds of contaminant concentrations at the mixing nodes before all processing units and sinks:

$$c_{m,\xi}^{\text{in}} \le \bar{C}_{m,\xi}^{\text{in}} \theta_{m,\xi}^{\text{in}} \qquad m \in \mathbb{M} \qquad \xi \in \mathbb{C} \tag{28}$$

where, $\bar{C}_{m,\xi}^{\text{in}}$ is the nominal value of maximum allowable concentration of contaminant ξ at the mixing node before unit m, and $\theta_{m,\xi}^{\text{in}}$ is the corresponding uncertain multiplier.

(2) The maximum outlet concentration limits of water-using units:

$$c_{u,\xi}^{\text{out}} \le \bar{C}_{u,\xi}^{\text{out}} \theta_{u,\xi}^{\text{out}} \qquad u \in \mathbb{U} \qquad \xi \in \mathbb{C} \tag{29}$$

where $\bar{C}_{u,\xi}^{\text{out}}$ represents the nominal value of maximum allowable outlet concentration of contaminant ξ for unit u, while $\theta_{u,\xi}^{\text{out}}$ is the corresponding uncertain multiplier.

(3) The maximum throughput limits of wastewater-treatment units:

$$f_t^{\text{in}} \le F_t \qquad t \in \mathbb{T} \tag{30}$$

where F^t represents the specified maximum throughput of unit t.

(4) The maximum supply limits of freshwaters:

$$\text{sr}_w \le S_w^{(1)} \qquad w \in \mathbb{W}_1 \tag{31}$$

where $S_w^{(1)}$ is the upper bound of the supply rate of freshwater source w.

Similarly, let us use another set of unified labels to represent the above inequality constraints:

$$\mathbb{K} = \{k \mid k \text{ is the label of an inequality process constraint}\} \tag{32}$$

Thus, the general form of these inequality constraints should be

$$g_k \le 0 \qquad k \in \mathbb{K} \tag{33}$$

or

$$g_k + s_k = 0 \qquad k \in \mathbb{K} \tag{34}$$

where $s_k \ge 0$ is a slack variable.

Complete Model Formulation. To facilitate formulation of a generalized model, all flows in the superstructure are assumed to be present initially. In a particular application, the flow rates of nonexistent branches in the given network should then be set to zero by introducing additional equality constraints. More specifically, a subset of the following constraints must be chosen on a case-by-case basis:

$$f_{w_1,d}^{W} = f_{w_1,p'}^{W} = 0 \quad w_1 \in \mathbb{W}_1 \quad d \in \mathbb{D} \quad p' \in \mathbb{P}_1 \tag{35}$$

$$f_{w_2,d}^{W} = f_{w_2,p'}^{W} = 0 \quad w_2 \in \mathbb{W}_2 \quad d \in \mathbb{D} \quad p' \in \mathbb{P}_2 \tag{36}$$

$$f_{p,p'} = f_{p,d}^{D} = 0 \quad p, p' \in \mathbb{P}_2 \quad d \in \mathbb{D} \tag{37}$$

For convenience, let us assign a new label to every constraint mentioned above. Since each constraint is associated uniquely with a branch in the superstructure, the set of all such labels can be defined as

$$\mathbb{J} = \{j \mid j \text{ is the label of a branch in the superstructure}\} \tag{38}$$

where, $\mathbb{J} = \mathbb{J}_0 \cup \mathbb{J}_1$ and

$$\mathbb{J}_0 = \left\{ \begin{matrix} j_0 \mid j_0 \text{ is the label corresponding to a} \\ \text{nonexistent branch in the given network} \end{matrix} \right\} \tag{39}$$

$$\mathbb{J}_1 = \left\{ \begin{matrix} j_1 \mid j_1 \text{ is the label corresponding to an existing} \\ \text{branch in the given network} \end{matrix} \right\} \tag{40}$$

Thus, a general form of these constraints used in a particular application should be written as

$$f_j = 0 \qquad j \in \mathbb{J}_0 \tag{41}$$

where f_j denotes a function of the flow rate of branch j, and this function is actually the same as its independent variable itself.

Thus, the generalized flexibility index model[7] can be formulated as

$$\min_{\delta,\mu_i,\nu_j,\lambda_k,s_k,y_k,x_i,z_n} \delta \tag{42}$$

subject to the constraints specified in eq 3, 27, 34, 41, and also those summarized below:

$$\sum_{k \in \mathbb{K}} \lambda_k = 1 \tag{43}$$

$$\sum_{i \in \mathbb{I}} \mu_i \frac{\partial h_i}{\partial \mathbf{z}} + \sum_{j \in \mathbb{J}} \nu_j \frac{\partial f_j}{\partial \mathbf{z}} + \sum_{k \in \mathbb{K}} \lambda_k \frac{\partial g_k}{\partial \mathbf{z}} = 0 \tag{44}$$

$$\sum_{i \in \mathbb{I}} \mu_i \frac{\partial h_i}{\partial \mathbf{x}} + \sum_{j \in \mathbb{J}} \nu_j \frac{\partial f_j}{\partial \mathbf{x}} + \sum_{k \in \mathbb{K}} \lambda_k \frac{\partial g_k}{\partial \mathbf{x}} = 0 \tag{45}$$

$$s_k - U(1 - y_k) \le 0 \qquad k \in \mathbb{K} \tag{46}$$

$$\lambda_k - y_k \le 0 \qquad k \in \mathbb{K} \tag{47}$$

$$\sum_{k \in \mathbb{K}} y_k \le N_z + 1 \tag{48}$$

$$\nu_j = 0 \qquad j \in \mathbb{J}_1 \tag{49}$$

where, μ_i, ν_j and λ_k are Lagrange multipliers; U represents a sufficiently large positive constant; N_z denotes the total number of control variables; $y_k \in \{0, 1\}$. Finally, notice that the last set of constraints in equation 49 are used to remove unnecessary terms, that is, those associated with the existing flows in $\mathbb{J}_1$, from the KKT conditions 44 and 45. This is due to the need to keep the same core conditions in the generalized model. As a result, it is only necessary to alter constraints 41 and 49 in each application.

Initialization Procedure

In this work, the GAMS modules DICOPT and BARON have been used to solve the aforementioned flexibility index models. Since the proposed model is written in a general code, only the constraints in eq 41 and eq 49 must be revised and then introduced in every optimization run. In addition, it has been well recognized that the starting point usually exerts a profound influence on the convergence process. A reliable initialization procedure has thus been developed to facilitate effective solution. This procedure is outlined below:

Step 1. Impose the additional constraints in eq 41 and eq 49 according to the given network configuration.

Step 2. Set the initial guesses of the flow rates in the existing branches. Specifically,

$$(f_j).l = \bar{f}_j \qquad j \in \mathbb{J}_1 \tag{50}$$

where, $(f_j).l$ denotes the initial value of f_j ($j \in \mathbb{J}_1$) and $\bar{f}_j$ represents the nominal flow rate of branch j in the given network.

Step 3. Compute the initial guesses of throughputs in water-using units, wastewater-treatment units, and mixers by substituting the initial guesses of branch flow rates obtained in Step 2 into eq 16 or 17. These initial throughputs are denoted as $(f_p^{\mathrm{out}}).l$ or $(f_p^{\mathrm{in}}).l$.

Step 4. Compute the initial guesses of freshwater consumption rates and effluent flow rates by substituting the initial guesses of branch flow rates obtained in Step 2 into eq 14 and eq 24. These initial guesses are denoted respectively as $(\mathrm{sr}_w).l$ for $w \in \mathbb{W}_1$ and $(f_d^{\mathrm{in}}).l$.

Step 5. Set the initial values of the flexibility index and all uncertain multipliers to be 1, that is,

$$(\delta).l = 1 \tag{51}$$

$$(\theta_{w,\xi}^{W}).l = 1 \qquad w \in \mathbb{W} \quad \xi \in \mathbb{C} \tag{52}$$

$$(\theta_{u,\xi}^{\mathrm{in}}).l = (\theta_{u,\xi}^{\mathrm{out}}).l = (\theta_{u,\xi}^{M}).l = 1 \qquad u \in \mathbb{U} \quad \xi \in \mathbb{C} \tag{53}$$

$$(\theta_{t,\xi}^{\mathrm{in}}).l = (\theta_{t,\xi}^{R}).l = 1 \qquad t \in \mathbb{T} \quad \xi \in \mathbb{C} \tag{54}$$

$$(\theta_{d,\xi}^{\mathrm{in}}).l = 1 \qquad d \in \mathbb{D} \quad \xi \in \mathbb{C} \tag{55}$$

Step 6. Determine the initial values of the inlet concentrations of processing units and sinks according to the nominal values of outlet concentrations of the processing units and concentrations of the water sources. Specifically, let

$$(c_{p,\xi}^{\mathrm{out}}).l = \bar{c}_{p,\xi}^{\mathrm{out}} \qquad p \in \mathbb{P}_2 \quad \xi \in \mathbb{C} \tag{56}$$

where, $\bar{c}_{p,\xi}^{\mathrm{out}}$ represents the nominal value of the concentration of ξ at the outlet of unit p.

The initial inlet concentrations can then be computed according to the contaminant balance equations. In other words, this task can be accomplished with the following equations:

$$(c_{p,\xi}^{\mathrm{in}}).l = [\sum_{p' \in \mathbb{P}_2} (f_{p',p}).l(c_{p',\xi}^{\mathrm{out}}).l + \sum_{w \in \tilde{\mathbb{W}}} (f_{w,p}^{W}).l\bar{C}_{w,\xi}]/(f_p^{\mathrm{in}}).l \qquad p \in \mathbb{P}_2 \quad \xi \in \mathbb{C} \tag{57}$$

$$(c_{d,\xi}^{\mathrm{in}}).l = [\sum_{p \in \mathbb{P}_2} (f_{p,d}^{D}).l(c_{p,\xi}^{\mathrm{out}}).l + \sum_{w \in \tilde{\mathbb{W}}} (f_{w,d}^{W}).l\bar{C}_{w,\xi}]/(f_d^{\mathrm{in}}).l \qquad d \in \mathbb{D} \quad \xi \in \mathbb{C} \tag{58}$$

where $\tilde{\mathbb{W}}$ is the set of water sources defined in eq 18; $(f_{p',p}).l$, $(f_{w,p}^{W}).l$, $(f_{p,d}^{D}).l$, and $(f_{w,d}^{W}).l$ represent the initial guesses of branch flow rates included in eqs 20 and 25.

In addition, it should be noted that the initial values produced with eq 57 can be replaced with those determined on the basis of the performance eqs 21−23. The corresponding convergence rate is equally acceptable in every application carried out so far.

Step 7. Estimate the initial guesses of slack variables defined in eq 34:

$$(s_k).l = -\bar{g}_k \qquad k \in \mathbb{K} \tag{59}$$

where, $(s_k).l$ denotes the initial guess of the kth slack variable and $\bar{g}_k$ is the function value of g_k evaluated at the nominal conditions.

Step 8. Initialize the binary variable y_k according to the definition of active constraint,[7] that is,

$$(y_k).l = \begin{cases} 1 & \text{if } |(s_k).l| \le \varepsilon \\ 0 & \text{otherwise} \end{cases} \tag{60}$$

where $k \in \mathbb{K}$ and ε is a small positive number to account for the truncation error in the computation.

Step 9. Generate the initial guesses of Lagrange multipliers for the inequality constraints, that is, λ_ks, according to the following two steps:

(1) Estimate the average value of all multipliers (λ^{ave}) and the distribution bound (λ^{dist}):

$$\lambda^{\mathrm{ave}} = \frac{1}{N_z + 1} \tag{61}$$

$$\lambda^{\mathrm{dist}} = \min(\lambda^{\mathrm{ave}}, 1 - \lambda^{\mathrm{ave}}) \tag{62}$$

(2) Set the initial guesses $(\lambda_k).l$ as

$$(\lambda_k).l = \begin{cases} \lambda^{\mathrm{ave}} + \Phi_{\mathrm{uni}}(-\lambda^{\mathrm{dist}}, +\lambda^{\mathrm{dist}}) & \text{if} \quad y_k = 1 \\ 0 & \text{if} \quad y_k = 0 \end{cases} \tag{63}$$

where, $k \in \mathbb{K}$ and $\Phi_{\mathrm{uni}}(-\lambda^{\mathrm{dist}}, +\lambda^{\mathrm{dist}})$ represents a generating function which yields a uniformly distributed random number in the interval $[-\lambda^{\mathrm{dist}}, +\lambda^{\mathrm{dist}}]$.

It is obvious that the initial guesses produced with the above procedure are very likely to satisfy eq 43.

Step 10. The upper bound of flexibility index δ can be estimated according to the calculation method presented in the sequel. For the sake of clarity, the rationale for adopting this approach is also provided.

From the definition of removal ratio, it is clear that its maximum value $R_{t,\xi}^{\max}$ should be one; that is,

$$R_{t,\xi}^{\max} = 1 \qquad t \in \mathbb{T} \quad \xi \in \mathbb{C} \tag{64}$$

Thus, the maximum value of corresponding uncertain multiplier $\overline{\theta_{t,\xi}^{R}}$ can be determined accordingly:

$$\overline{\theta_{t,\xi}^{R}} = 1/\bar{R}_{t,\xi} \qquad t \in \mathbb{T} \quad \xi \in \mathbb{C} \tag{65}$$

where, $\bar{R}_{t,\xi}$ is the nominal value of removal ratio $R_{t,\xi}$. To ensure feasibility, a conservative strategy is to select the upper bound of flexibility index in such a way that

$$(\delta).\mathrm{up} = \min_{t \in \mathbb{T}, \xi \in \mathbb{C}} \frac{\overline{\theta_{t,\xi}^{R}} - 1}{\Delta\theta_{t,\xi}^{R+}} \tag{66}$$

where $(\delta).\mathrm{up}$ is the upper bound of flexibility index used in the optimization run and $\Delta\theta_{t,\xi}^{R+}$ is the expected deviation of uncertain multiplier $\theta_{t,\xi}^{R}$ from its nominal value in the positive direction.

Case Studies

Two examples are presented below to demonstrate the usefulness of the generalized flexibility index model and the proposed initialization procedure:

Example 1. Let us first consider the revamp designs of an existing water network shown in Figure 2, which consists of a

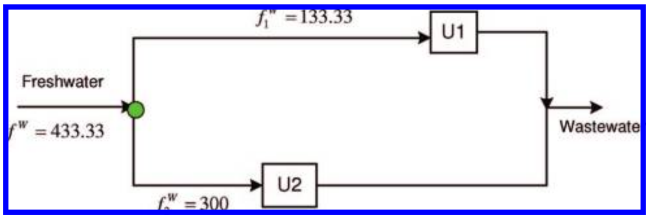

Figure 2. Nominal water network in Example 1.

Table 1. Design Specifications of Water-Using Units in Example 1

unit	$\bar{C}^{\text{in}}$ (ppm)	$\bar{C}^{\text{out}}$ (ppm)	mass load (kg/h)	limiting flowrate (ton/h)
$u1$	70	170	20	200
$u2$	20	120	30	300

Table 2. Nominal Operating Conditions of Water-Using Units in Example 1

unit	$\bar{C}^{\text{in}}$ (ppm)	$\bar{C}^{\text{out}}$ (ppm)	mass load (kg/h)	flowrate (ton/h)
$u1$	20	170	20	133.33
$u2$	20	120	30	300

single water source and two water-using units. The design specifications and nominal operating conditions of the water-using units in the original design are provided in Tables 1 and 2, respectively. Notice that only one key contaminant is adopted in the network design. The maximum allowable freshwater supply rate is 433.33 ton/h (which is the minimum freshwater usage when the opportunities of wastewater reuse is ignored) and the nominal contaminant concentration in freshwater is 20 ppm. Notice that a splitter is located at the source and it is marked by a small circle in Figure 2. The split ratios of its two branch streams can be adjusted to compensate for external disturbances during operation. It is assumed in this example that the maximum inlet and outlet contaminant concentrations of unit 1, that is, C_1^{in} and C_1^{out}, and the maximum contaminant concentration at the outlet of unit 2, that is, C_2^{out}, may vary with the ambient temperature. The corresponding uncertain multipliers are referred to as θ_1, θ_2, and θ_3, respectively. It is further assumed that

$$\Delta\theta_1^- = \Delta\theta_2^- = \Delta\theta_3^- = 0.04$$

$$\Delta\theta_1^+ = \Delta\theta_2^+ = \Delta\theta_3^+ = 0.05$$

Notice that $\theta_1^N = \theta_2^N = \theta_3^N = 1$. A total of 19 variables (including 3 binary variables) are needed to formulate the corresponding flexibility index model. This model was easily solved with GAMS modules (version 22.4)[12] on a HP Compag DC7700 convertible minitower. The default NLP solver in GAMS is CONOPT3 and MIP solver is CPLEX, while DICOPT and BARON are both adopted to solve MINLP for comparison and validation purposes.[14] The optimization computation converged within 1 s and nearly no initialization steps were required for this simple problem. It can be found from the optimal solution that the flexibility index in this case is zero, which is clearly undesirable. The following steps were then taken to evaluate the benefits of introducing additional design changes:

(1) Attach auxiliary pipeline(s): An additional pipeline from $u2$ to $u1$ was first added to the original network (see Figure 3), while the upper limit of freshwater usage was still kept unchanged. As a result, the total number of variables in the corresponding model became 20. It was found that the flexibility index could be increased to 1.6026 with the aforementioned auxiliary pipeline, and the corresponding optimum solution is presented in Table 3. Since $\delta > 1$, it is clear that the improved network design is operable or has enough flexibility to counteract all possible disturbances by adjusting the control variables. From the above optimum solution, it can also be observed that the most constrained point in design is located at where every uncertain multiplier reaches its lower bound:

$$1 - \delta \times \Delta\theta_i^- = 1 - 1.6026 \times 0.04 = 0.936$$

where, $i = 1, 2, 3$. This finding is of course consistent with our intuitive prediction.

Other possible auxiliary pipelines, such as those from $u1$ to $u2$ and from water source to sink, were excluded from consideration. Notice that the former design change obviously violates the optimality conditions of water network design.[15] More specifically, the outlet contaminant concentration of unit $u1$ should reach its upper bound (when the total freshwater usage of the network is to be minimized) which is larger than that of unit $u2$, and the water reuse stream from $u1$ to $u2$ can only increase the total freshwater usage of the network. On the other hand, since the freshwater cannot be directed to the water-using units with a source-to-sink pipeline and no upper limit is imposed upon the contaminant concentration in effluent, it is clearly unnecessary to consider the latter structural modification.

(2) Relax upper bound of freshwater usage: On the basis of the improved configuration obtained in the previous step, the generalized flexibility index model was also solved repeatedly for different levels of maximum freshwater supply rate. From the corresponding results presented in Table 4 and Figure 4, it is obvious that the flexibility index of this water network increases almost linearly with the supply limit of freshwater. Furthermore, 420 ton/h is the minimum freshwater capacity for ensuring adequate operational flexibility under the influences of anticipated uncertain disturbances.

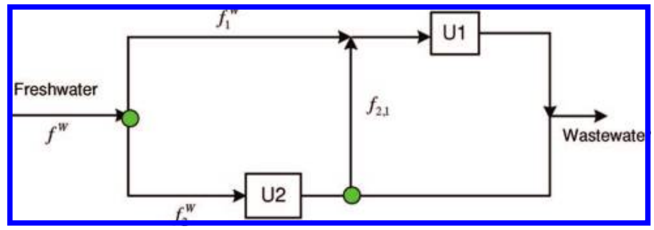

Figure 3. Improved water network in Example 1.

Table 3. Optimum Solution Obtained in Example 1

unit	C^{in} (ppm)	C^{out} (ppm)	flowrate (ton/h)
$u1$	65.51	159.10	213.70
$u2$	20	112.31	325.00

Table 4. Flexibility Index Values Obtained with Different Freshwater Levels in Example 1

freshwater usage (ton/h)	flexibility index δ
400	0
410	0.51
420	0.99
425	1.23
430	1.45
433.33	1.6026
440	1.89

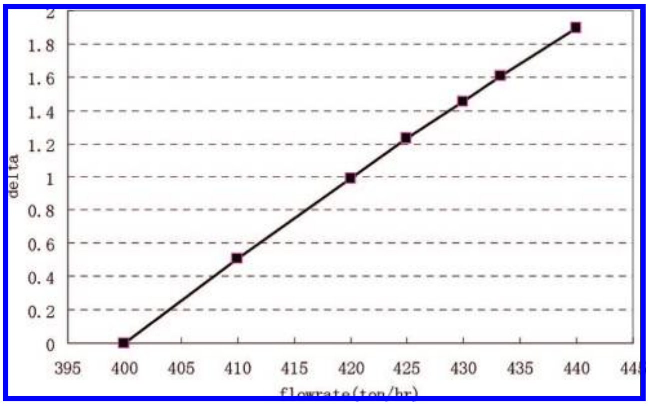

Figure 4. Impact of increasing freshwater supply capacity on flexibility index in Example 1.

Table 5. Stream Data of Water Sources in Example 2

	F^{W} (ton/h)	$\bar{C}_w$ (ppm)
$w1$	∞	0.1
$w2$	30	150.0

Table 6. Design Specifications of Water-Using Units in Example 2

unit	C_{max}^{in} (ppm)	C_{max}^{out} (ppm)	F_{lim}^{in} (ton/h)	$\bar{M}$ (kg/h)
$u1$	1	101	40	4.0
$u2$	80	240	35	5.6
$u3$	50	200	30	4.5

Table 7. Design Specifications of Wastewater-Treatment Units in Example 2

Unit	C_{max}^{in} (ppm)	F_{max}^{in} (ton/h)	removal ratio $\bar{R}$
$t1$	185	125	0.9
$t2$	200	135	0.8

Example 2. Let us next consider a grass-root design problem concerning one freshwater source, one secondary water source, three water-using units, two wastewater treatment units, and a wastewater sink. The nominal stream data of water sources are provided in Table 5. The design specifications of water-using units and wastewater-treatment units are given in Table 6 and Table 7, respectively. It is also assumed that there is a maximum concentration limit of 10 ppm imposed at the sink.

Various different alternative cost-optimal network designs can be first obtained with the traditional mathematical programming approach on the basis of different versions of the superstructure.[16,17] In this example, these networks are generated for use as the "nominal" designs for the subsequent flexibility analysis. Four such candidates are shown in Figures 5−8, and they are referred to as designs I−IV, respectively. Notice that more can be produced with the same approach if necessary. The optimal operating conditions of the water-using and wastewater-treatment units in the above four designs are provided in Tables 8−11, respectively. The design objectives in all cases are the same, that is, minimization of the freshwater consumption rate. The superstructures used for producing the first two networks do not include mixers, while only one is adopted in the latter two. From Figure 5 and 6, notice that the same level of freshwater usage, 26.489 ton/h, is required in the first two designs. A total of 15 stream branches and 8 splitters are included in design I, while 12 stream branches and 5 splitters are needed in design II. From Figure 7 and 8, notice that much less freshwater (8.384 ton/h) is needed in the last two designs. The reduction of freshwater requirement is achieved at the cost of installing the self-recycle stream around treatment unit $t2$. Five splitters are adopted in both designs III and IV, while 12 and 13 branches are present in these two networks, respectively.

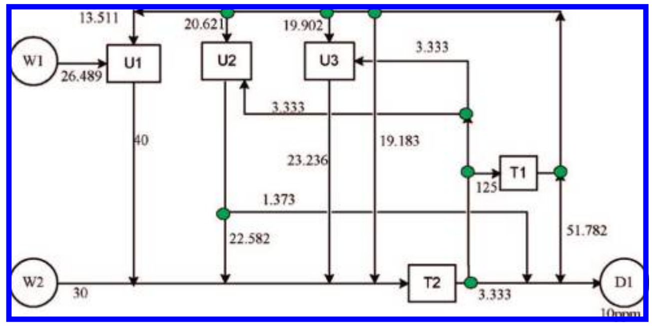

Figure 5. Design I in Example 2.

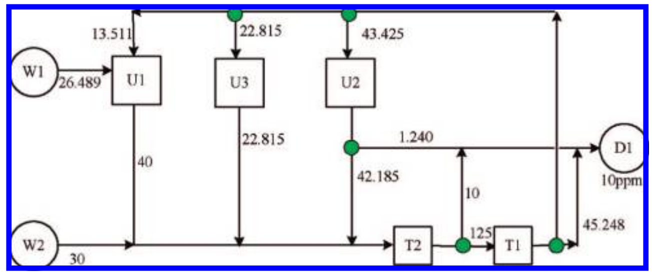

Figure 6. Design II in Example 2.

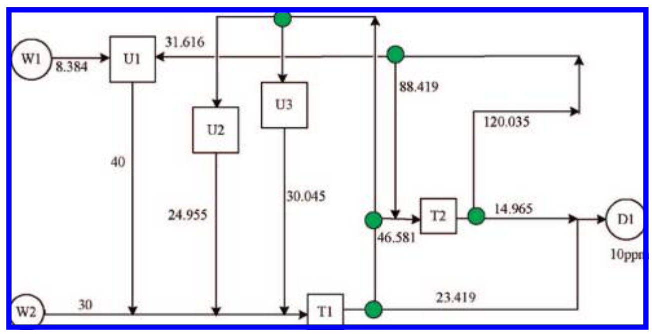

Figure 7. Design III in Example 2.

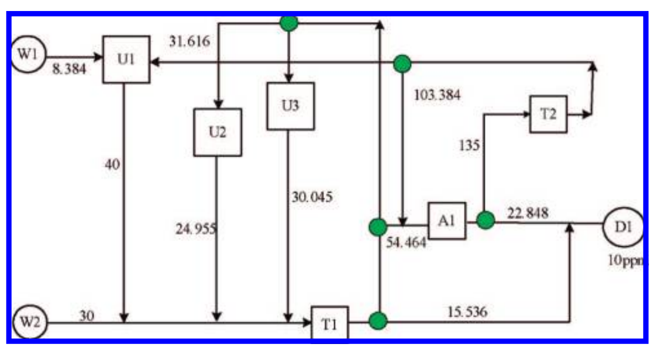

Figure 8. Design IV in Example 2.

It is assumed in this example that the external disturbances during normal operation may cause three types of design parameters to fluctuate: (1) the contaminant concentration in freshwater, (2) the mass load of every water-using unit, and (3) the removal ratio of every wastewater-treatment unit. Thus, the following uncertain multipliers were introduced into the general-

Table 8. Nominal Operating Conditions of All Units in Design I for Example 2

unit	*u*1	*u*2	*u*3	*t*1	*t*2	*d*1
flowrate(ton/h)	40.000	23.955	23.236	125.000	135.000	56.489
c^{in} (ppm)	1.000	6.226	6.334	27.644	138.220	10.000
c^{out} (ppm)	101.000	240.000	200.000	2.764	27.644	

Table 9. Nominal Operating Conditions of All Units in Design II for Example 2

unit	*u*1	*u*2	*u*3	*t*1	*t*2	*d*1
flowrate(ton/h)	40.000	43.425	22.815	125.000	135.000	56.489
c^{in} (ppm)	1.000	2.764	2.764	27.644	138.220	10.000
c^{out} (ppm)	101.000	131.723	200.000	2.764	27.644	

Table 10. Nominal Operating Conditions of All Units in Design III for Example 2

unit	*u*1	*u*2	*u*3	*t*1	*t*2	*d*1
flowrate(ton/h)	40.000	24.955	30.045	125.000	135.000	38.384
c^{in} (ppm)	1.000	15.598	15.598	155.983	6.193	10.000
c^{out} (ppm)	101.000	240.000	165.375	15.598	1.239	

Table 11. Nominal Operating Conditions of All Units in Design IV for Example 2

unit	*u*1	*u*2	*u*3	*t*1	*t*2	*a*1	*d*1
flowrate (ton/h)	40.000	24.955	30.045	125.000	135.000	157.848	38.384
c^{in} (ppm)	1.000	15.598	15.598	155.983	6.193	6.193	10.000
c^{out} (ppm)	101.000	240.000	165.375	15.598	1.239	6.193	

Table 12. Flexibility Indices of Designs I and II in Example 2

freshwater usage (ton/h)	26.489	30	35	38	40
design I	0	0.320	0.825	1.153	1.383
design II	0	0.320	0.825	1.153	1.402

Table 13. Flexibility Indices of Designs III and IV in Example 2

freshwater usage (ton/h)	8.384	10	15	18	26.489	30	35
design III	0	0.072	0.3047	0.3744	0.3839	0.3874	0.3920
design IV	0	0.072	0.3047	0.3744	0.3839	0.3874	0.3920

ized flexibility index model:

$$0.9 \le \theta_1^W \le 1.1 \tag{67}$$

$$0.85 \le \theta_1^M, \theta_2^M, \theta_3^M \le 1.15 \tag{68}$$

$$0.97 \le \theta_1^R, \theta_2^R \le 1.03 \tag{69}$$

Notice that these multipliers have been defined in eq 20, 21, and 22, respectively, and the second subscripts (ξ) are dropped since there is only one key contaminant considered in this example.

All optimization runs in this example were carried out with BARON, the DICOPT solver was used only when convergence difficulties occurred. The CPU time needed for completing each run was usually within 100 s. If the upper limits of freshwater supply rates in the aforementioned four networks are kept at their respective nominal levels, it is not surprising to discover that the corresponding flexibility indices are zero. The operational flexibility in these four designs can certainly be improved by raising the upper limit of freshwater usage (see Tables 12 and 13). For illustration clarity, the same results are also plotted in Figures 9 and 10, respectively. The flexibility index can be improved to 1 when the freshwater usage is increased from 26.489 ton/h to about 38 ton/h for both design I and design II.

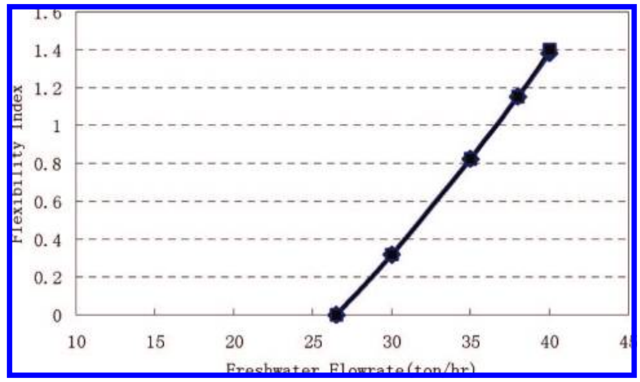

Figure 9. Impact of increasing freshwater supply capacity on flexibility index of designs I and II in Example 2.

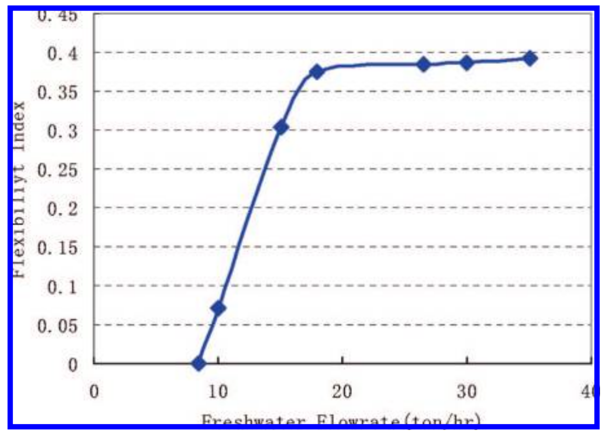

Figure 10. Impact of increasing freshwater supply capacity on flexibility index of designs III and IV in Example 2.

This increase in freshwater consumption can be regarded as the cost for counteracting the aforementioned uncertain disturbances. Although the flexibility index of design I or II can be approximated by a linear function (see Figure 9), this index for designs III and IV tends to reach a constant upper bound (see Figure 10). It can thus be deduced that designs I and II are superior in the sense that they are capable of sustaining unexpected disturbances in practical operations. In addition, it is interesting to note that the flexibility index does not necessarily increase with the number of control variables. Thus, there is really no need to introduce auxiliary pipelines or other structural changes into the cost-optimal designs for the present problem since it is always possible to generate more candidate network configurations for grassroots design.

Conclusions

A MINLP-based design procedure is developed in this work for assessing and improving the operational flexibility of existing water networks under uncertain disturbances. Specifically, a generalized flexibility index model and its initialization procedure are proposed for evaluating the benefits of introducing additional design options, that is, relaxation of the upper limit of freshwater supply rate and incorporation of structural modifications. It has been shown in the case studies that this approach is feasible and efficient. Furthermore, the following conclusions can also be drawn from the optimization results obtained in the examples:

1. The flexibility index of any optimal water network is zero when the minimum freshwater usage is used.

2. For an existing water network, its flexibility index can be increased when freshwater usage is relaxed, and this increase is dependent upon the network structure.

3. The most constrained point of water network under disturbances is the point where the concentration of freshwater and the mass load of water-using unit reaches their upper bound while the removal ratios of treatment units and the allowed maximum inlet and outlet concentration approaches their lower bound. This finding may be useful for selecting structural changes in revamp studies.

Acknowledgment

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Nomenclature

(1) Sets, Parameters, and Variables
δ = variable of flexibility index
ε = a real scalar
θ = set of uncertain parameters
Θ = parameter space of θ
μ, ν = Lagrange multiplier of equality constraint
λ = Lagrange multiplier of inequality constraint
$\mathbb{A}$ = set of mixer units
C, c = concentration
$\mathbb{C}$ = set of contaminants
$\mathbf{d}$ = vector of design variables
$\mathbb{D}$ = set of water sinks
f = flowrate
$\mathbf{g}$ = vector of inequality constraints
$\mathbf{h}$ = vector of equality constraints
$\mathbb{I}$ = index set of equality constraint
$\mathbb{J}$ = set of branches in the superstructure
$\mathbb{K}$ = index set of inequality constraint
M = mass load of water-using unit
$\mathbb{M}$ = union set of $\mathbb{U}$, $\mathbb{T}$, and $\mathbb{D}$
$\mathbb{P}_1$ = union set of $\mathbb{U}$ and $\mathbb{A}$
$\mathbb{P}_2$ = union set of $\mathbb{U}$, $\mathbb{T}$, and $\mathbb{A}$
s = slack variable
$\mathbb{T}$ = set of wastewater treatment units
U = a big enough positive number
$\mathbb{U}$ = set of water-using units
$\mathbb{W}$ = set of water sources
$\mathbf{x}$ = set of state variables
y = binary variable
$\mathbf{z}$ = set of control variables
(2) Superscripts
ave = average
dist = disturbance
M = mass load
out = outlet
W = water source
D = wastewater sink
in = inlet
N = nominal
R = removal ratio
(3) Subscripts
ξ = contaminant
a = mixer
i = equality constraint
m = process unity in $\mathbb{M}$
t = treatment unit
w = water source
d = water sink
k = inequality constraint
p, p' = process unit in $\mathbb{P}$
u = water-using unit

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