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Efficient Flexibility Assessment Procedure for Water Network Designs

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S Supporting Information

ABSTRACT: A *new* nonlinear programming (NLP) formulation of the conventional flexibility index model (Swaney and Grossmann, 1985) has been developed in this work for flexibility analysis of single-contaminant water networks. Since this improved model is constructed on the basis of a single critical point instead of the entire region of uncertain parameters, the iterative optimization process converges at a much faster rate. A systematic flexibility assessment procedure has also been devised to analyze and modify a given network so as to achieve the desired level of operational resiliency. Specific design steps are followed sequentially to check the feasibility of a nominal design and to improve its flexibility index by (1) relaxing the upper limit of freshwater capacity and/or (2) adding new pipelines and/or removing existing ones. The effectiveness of the proposed approach is demonstrated with two examples in this paper.

1. INTRODUCTION

The importance of water to most industrial processes cannot be overemphasized. It is commonly used in large quantities as reagents, mass-separating agents, and heat-transfer media in various water-using units.[1] With the scarcity of freshwater resources and increasingly stringent environmental regulations, water integration becomes a popular option in process design for minimizing the volumes of consumed and discharged water.[2,3] Since the configuration of any integrated water network is inevitably quite complex, its feasibility in practice is often questionable. Therefore a thorough flexibility analysis should be performed at the design stage to ensure that the water utilization system under consideration is operable even when the actual operating conditions deviate from those assumed for nominal design.[4,5]

In most existing studies on water network design, it is a common practice to assume that the values of process parameters are fixed and well-defined. These process parameters could include the maximum freshwater supply rate, the mass loads of water using units, the removal ratios of wastewater treatment units, and the upper limits of pollutant concentrations at the inlet and/or outlet of processing units, etc. Since the actual operating conditions may fluctuate over time, the aforementioned fixed parameter values can only be viewed as those estimated under nominal conditions. Furthermore, such estimates of the nominal parameters themselves may also be inaccurate due to the designer's incomplete/incorrect knowledge of the given system. Consequently, the actual parameter values should be considered as uncertain and they may be located anywhere within a finite region in the parameter space. A water network designed solely on the basis of nominal parameters may not be flexible enough to cope with all possible changes during operation.[1] The usual way to account for uncertainties is by overdesign, for example, the capacities of freshwater supply and branch flows can be increased to higher-than-nominal levels. Since the overdesign levels are traditionally determined in an ad hoc fashion according to past experiences, a quantitative assessment method is obviously needed in this situation to facilitate more rational decisions.

In general, the term "flexibility" is considered as the capability of a process to function adequately over a given range of uncertain conditions.[6,7] There are in fact very few reported studies devoted specifically to the analysis and design of resilient water networks. Tan and Cruz[8] 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[9] developed a three-step procedure to design water networks under uncertain operating temperatures and pressures. The impacts of uncertainties were evaluated with a scenario-based approach; that is, the uncertain parameters take on different values in different design cases. Karuppiah and Grossmann[10] studied a similar problem, and proposed a spatial branch-and-cut algorithm to locate the global optimum. Tan, Foo, and Manan[1] used the Monte Carlo simulation techniques to access the vulnerability of water networks which are subject to noisy mass loads. Zhang, Feng, and Qian[11] suggested the use of 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.

Recently, Chang *et al.*[4] developed a generalized mixed integer nonlinear programming model for assessing and improving the operational flexibility of water network design. In their work, the *flexibility index model* proposed by Swaney and Grossmann[12] has

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been modified and formulated in a generalized format to determine a quantitative measure of the operational resiliency of any given network. Their MINLP model was utilized in a trial-and-error fashion to enhance the operational flexibility by relaxing the allowed freshwater consumption rate and/or installing auxiliary pipelines. Later, Riyanto and Chang[5] proposed a heuristical strategy based on *active constraints* to improve the operation flexibility of existing water networks by inserting/deleting pipeline connections and adding/replacing treatment units. Since the model they adopted was a mixed integer nonlinear program (MINLP), the corresponding iterative solution processes often required elaborate initialization schemes and/or significant computation resources. To circumvent this drawback, a simplified *new* nonlinear programming (NLP) model is developed in this study to perform the calculation of flexibility index efficiently. Since such model is built on the basis of *a single critical point* (which was reported in Chang et al.[4]) instead of the entire uncertain region in the parameter space, the convergence rate of the optimization computation becomes much faster.

Furthermore, since it is generally recognized that the available design strategies are not mature enough for generating cost-optimal water networks which are also resilient,[11] a comprehensive flexibility assessment procedure has also been developed in this work to achieve this purpose. In particular, if an economical network design fails to pass the feasibility test, two remedial options have been used in the present work to improve its operational flexibility: (1) relaxation of the overdesign level of freshwater supply system and (2) installation of auxiliary pipelines and/or elimination of original ones. In the former case, a modified version of the aforementioned NLP model can be formulated to determine the minimum level of the upper limit of freshwater supply rate so as to ensure a flexibility index value of exactly 1. If this remedial measure is not feasible, another MINLP model can then be constructed on the basis of the proposed NLP model to automatically revise the network connections so as to raise the flexibility index level to be just 1.

The remaining paper is organized as follows. A concise problem statement is first provided in the next section. Next the general framework of the improved flexibility index model is given in section 3 and the corresponding detailed formulation is provided in section 4. Alternative forms of this model can be constructed to perform various different tasks in the flexibility assessment procedure. These modified versions are presented in section 5. To demonstrate the effectiveness of the proposed new approach, the numerical results obtained in two case studies are described in section 6. Finally, concrete conclusions are drawn in the last section.

2. PROBLEM STATEMENT

As mentioned previously, the primary objective of the present work is to develop a set of systematic methods to analyze and then enhance the operational resiliency of any given water-network design for a *continuous* chemical process. This design should include specifications of (1) the network configuration, (2) the freshwater consumption rate and the overdesign level of the corresponding supply system, (3) the water flow rate of every branch in the network and its overdesign level, (4) the effluent flow rates, (5) the throughput of every water using and wastewater treatment unit, and (6) the contaminant concentrations at the sinks and also at the inlets and outlets of all processing units. In this study, some of the process parameters are considered to be available and can be treated as constants for the subsequent flexibility analysis, that is, the flow rates of secondary water, the throughput limits of wastewater treatment units, and the upper bounds of pollutant concentrations at the sinks. It is also assumed that the remaining process parameters, that is, the water source qualities, the mass loads of water using units, and their maximum allowable inlet and outlet pollutant concentrations, and the removal ratios of wastewater treatment units and the upper bounds for their inlet pollutant concentrations, may be uncertain and an estimate of the corresponding uncertain region in the parameter space can be obtained in advance.

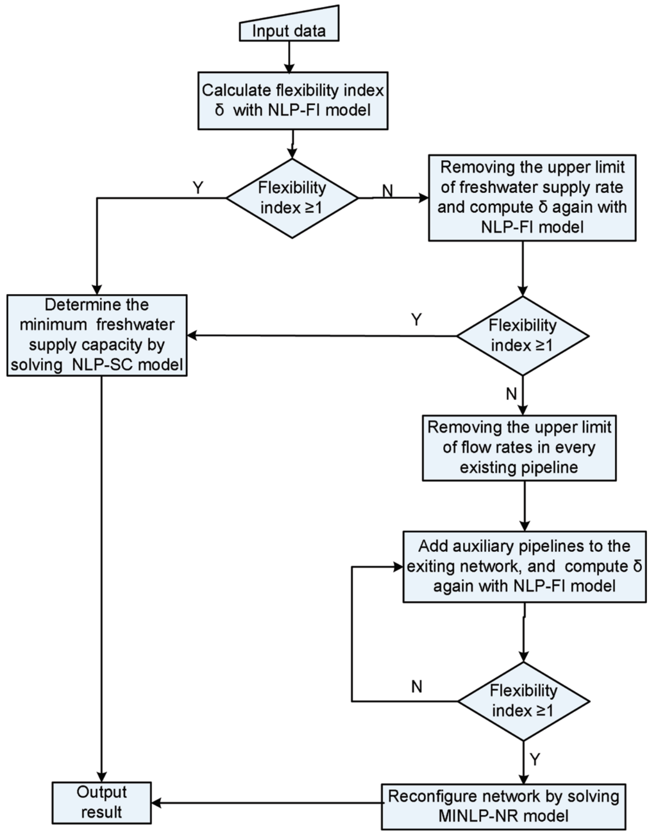

Figure 1. Flexibility assessment procedure.

It is our intention to answer the following questions in sequence with an improved version of the flexibility index model or its alternative forms: (1) Is the given water network design operable in realistic environment? (2) If not, is it possible to make the design flexible enough simply by increasing the overdesign level of freshwater supply system and what should be its minimum level? (3) If the above remedial measure is not successful, is it possible to achieve the desired flexibility level by modifying the network configuration and how?

This flexibility assessment procedure can be summarized with the flowchart presented in Figure 1.

3. GENERAL FRAMEWORK OF IMPROVED FLEXIBILITY INDEX MODEL

The flexibility index model developed by Swaney and Grossmann[12] has been adopted in this work as a basic tool for the aforementioned assessment tasks. Its framework is outlined below to facilitate subsequent illustration of detailed model formulation. First of all, it should be noted that the original flexibility index model can be expressed in a general form as

$$F = \max \delta$$
$$\text{s.t.} \quad h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) = 0, \quad i \in \mathbb{I} \tag{1}$$

$$\min_{\mathbf{z}} \max_{j \in \mathbb{J}} g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) \le 0 \tag{2}$$

$$\Theta(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\}, \quad \delta \ge 0 \tag{3}$$

where, $h_i = 0$ ($i \in \mathbb{I}$) denotes a system of equations characterizing mass balances in the water network and also operation performances of the processing units; $g_j \le 0$ ($j \in \mathbb{J}$) represents the set of inequalities for stipulating the design specifications and physical limits which must be enforced to ensure feasible operation. Notice that **d** is a vector of fixed model parameters which define the network structure and equipment sizes. Their values should be made available at the design stage and kept as constants during plant operation. In particular, these parameters include the maximum freshwater supply rate, the maximum throughputs of all water using and wastewater treatment units, the maximum allowable limits of all branch flows, and the upper bounds of pollutant concentrations in effluents. On the other hand, θ is the vector of uncertain parameters, and an exhaustive list of such parameters have already been given in the previous section. The process variables can be classified into two groups, that is, the control variables in vector **z** and the state variables in vector **x**. Since dim **x** = dim **h**, the vector size of **z** can be considered as the degree of freedom during plant operation. In other words, the control variables can be adjusted online for different realizations of the uncertain parameters θ. 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 of 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 region Θ in the parameter space can be defined according to eq 3. In this definition, θ^N represents a vector of parameter values from which the nominal design can be 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. It is also assumed in this study that these parameters can vary *independently* within their specified intervals.

Clearly, it is difficult to solve the aforementioned model. This is mainly due to eq 2, which in general results in a nondifferentiable optimization problem.[6] Although the active-constraint method was implemented successfully in our previous study,[4] the required computation load can still be quite heavy. An alternative approach, such as, the vertex method,[13] has been adopted in this work to reduce the solution effort. Specifically, only the parameter values corresponding to vertices of the uncertain region $\Theta(\delta)$ can be used for computing the flexibility index; that is,

$$F = \min_{k \in \mathbb{V}} \delta^k$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$ ($k \in \mathbb{V}$); that is,

$$\delta^k = \max_{\delta, \mathbf{z}} \delta$$

$$\text{s.t.} \quad h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) = 0, \quad i \in \mathbb{I} \tag{4}$$

$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \theta) \le 0, \quad j \in \mathbb{J} \tag{5}$$

$$\theta = \theta^N + \delta\Delta\theta^k, \quad \delta \ge 0 \tag{6}$$

It should be noted that all vertices still have to be checked according to this original version of vertex method. However, it has been found in our previous work[4] that the most constrained point (or the critical point) of a water network design can be associated with an upper or lower limit of each uncertain parameter on the basis of physical insights. These particular locations are (1) the upper bounds of (i) the mass loads of water using units and (ii) the pollutant concentrations at the primary and secondary sources; (2) the lower bounds of (i) the removal ratios of wastewater treatment units, (ii) the allowed maximum inlet and outlet pollutant concentrations of water using units, (iii) the allowed maximum inlet pollutant concentration of wastewater treatment units.

The flexibility index of a water network can thus be determined on the basis of this most constrained point alone. Such an improved model for computing flexibility index is referred to as the NLP-FI model in the present paper. It should be pointed out that the validity of this approach has already been confirmed empirically with extensive case studies in our previous studies.[4] Specifically, the original flexibility index model proposed by Swaney and Grossmann[12] has been modified and formulated in a general format to evaluate the impacts of introducing various modifications (i.e., relaxing the upper limit of freshwater supply rate and/or modifying the network structure of the given design) to the existing designs, the flexibility indices of 31 cases (7 cases in Example 1 and 24 cases in Example 2) were calculated and reported by Chang et al.[4] The suggested critical directions were confirmed in all these cases (and in additional unreported cases) without exception. Finally, notice that a more specific justification can also be found in the next section.

4. DETAILED MODEL FORMULATION

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 structures under consideration. As mentioned previously, it is our purpose to maximize the value of δ at the most constrained point with this model. The detailed model constraints are presented below:

4.1. 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.[3] In its original form, a distinct label is assigned to each water using unit, wastewater treatment unit, water source, and sink; that is,

$$\mathbb{U} = \{u | u \text{ is the label of a water using unit in the plant}; \; u = 1, 2, \cdots, N_U\} \tag{7}$$

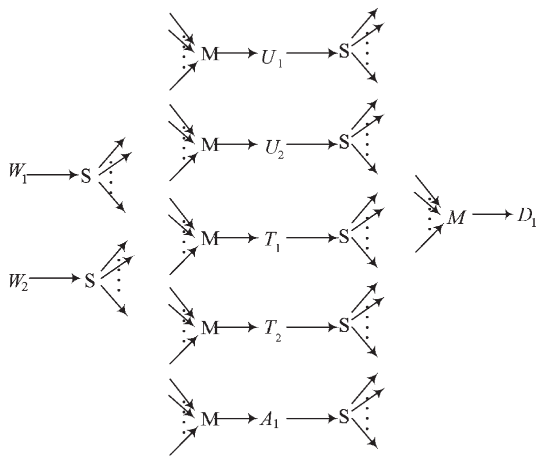

Figure 2. Superstructure of water network.

$$\mathbb{T} = \{t|t \text{ is the label of a water-treatment unit in the plant}; \quad t = 1, 2, \cdots, N_T\} \tag{8}$$

$$\mathbb{W} = \{w|w \text{ is the label of water source}; \quad w = 1, 2, \cdots, N_W\} \tag{9}$$

$$\mathbb{D} = \{d|d \text{ is the label of water sink}; \quad d = 1, 2, \cdots, N_D\} \tag{10}$$

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

$$\mathbb{W}_1 = \{w_1|w_1 \text{ is the label of a freshwater source}; \quad w_1 = 1, 2, \cdots, N_{W_1}\} \tag{11}$$

$$\mathbb{W}_2 = \{w_2|w_2 \text{ is the label of a secondary source}; \quad w_2 = 1, 2, \cdots, N_{W_2}\} \tag{12}$$

where, $N_W = N_{W_1} + N_{W_2}$. 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,

$$\mathbb{A} = \{a|a \text{ is the label of a mixer unit in the plant}; \quad a = 1, 2, \cdots, N_A\} \tag{13}$$

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 $\mathbb{U}$ 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 illustrated by the example given in Figure 2, in which one freshwater source ($\mathscr{W}_1$), one secondary source ($\mathscr{W}_2$), two water using units ($\mathscr{U}_1$ and $\mathscr{U}_2$), two wastewater treatment units ($\mathscr{T}_1$ and $\mathscr{T}_2$), one mixer ($\mathscr{A}_1$) and a sink are involved and the symbols $\mathscr{S}$ and $\mathscr{M}$ denote the splitting and mixing node, respectively.

4.2. Process Constraints. Without loss of generality, the following assumptions are adopted in this paper for illustration convenience: (1) The water network works continuously. (2) It is possible to consider only one key contaminant in the mass balance equations. (3) The possibility of water gain or loss in each processing unit is excluded. (4) Contaminant concentration in every water stream is very small and thus the effects of its variation on flow rate are negligible.

Let us also introduce the following set definitions to facilitate concise model formulation:

$$\mathbb{P}_1 = \mathbb{U} \cup \mathbb{A} \tag{14}$$

$$\mathbb{P}_2 = \mathbb{U} \cup \mathbb{T} \cup \mathbb{A} \tag{15}$$

A set of equality and inequality constraints can then be formulated to satisfy process requirements according to Figure 2. These constraints are presented as follows.

4.2.1. Water sources. At the splitting nodes originated from primary and secondary water sources, the generalized flow balance equations can be written as

$$\mathrm{sr}_w = \sum_{p \in \mathbb{P}_\ell} f^{\mathrm{W}}_{w,p} + \sum_{d \in \mathbb{D}} f^{\mathrm{W}}_{w,d} \quad w \in \mathbb{W}_\ell \tag{16}$$

where, $\ell \in \{1, 2\}$; $\mathrm{sr_w}$ is the total water supply rate from source w; $f^{W}_{w,p}$ and $f^{W}_{w,d}$ denote the flow rates of water (from source w) which are consumed by processing unit p and sink d, respectively. Since the secondary water sources[3] must be completely consumed and their supply rates are assumed to be constants in this study, the following constraints should also be imposed

$$\mathrm{sr}_w = S^{(2)}_w \quad w \in \mathbb{W}_2 \tag{17}$$

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

4.2.2. Processing Units. The generalized water balance equation at the splitting node from the outlet of a processing unit p can be expressed as

$$f^{\mathrm{out}}_p = \sum_{p' \in \mathbb{P}_2} f_{p,p'} + \sum_{d \in \mathbb{D}} f^{\mathrm{D}}_{p,d} \qquad p \in \mathbb{P}_2 \tag{18}$$

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'; $f^{\mathrm{D}}_{p,d}$ is the flow rate of wastewater generated by unit p and sent to sink d.

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

$$f^{\mathrm{in}}_p = \sum_{p' \in \mathbb{P}_2} f_{p',p} + \sum_{w \in \tilde{\mathbb{W}}} f^{\mathrm{W}}_{w,p} \quad p \in \mathbb{P}_2 \tag{19}$$

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; $f^{\mathrm{W}}_{w,p}$ is the water flow rate from source w to unit p and

$$\tilde{W} = \begin{cases} \mathbb{W}_1 \cup \mathbb{W}_2 & \text{if} \quad p \in \mathbb{U} \cup \mathbb{A} \\ \mathbb{W}_2 & \text{if} \quad p \in \mathbb{T} \end{cases} \tag{20}$$

Since the water loss or gain in every processing unit is assumed to be negligible in this study, the corresponding mass balance can be

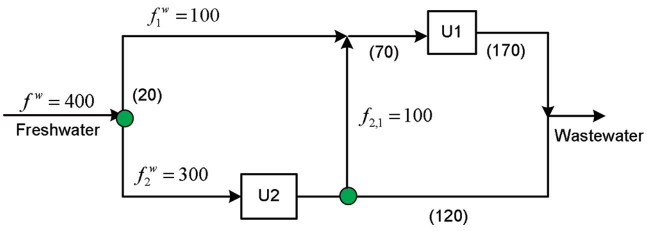

Figure 3. Nominal water network in example 1.

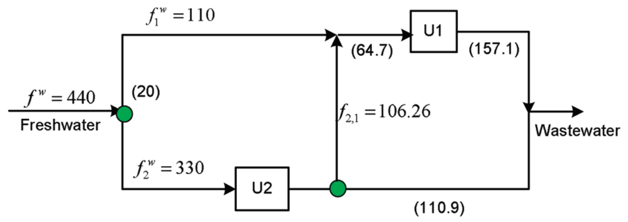

Figure 4. Critical water network in example 1.

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

unit	$\overline{C}^{in}$ (ppm)	$\overline{C}^{out}$ (ppm)	mass load (kg/h)	limiting flow rate (ton/h)
u1	70	170	20	200
u2	50	120	30	300

Table 2. Comparison of main results in Example 1

		Overdesign			
step	model	freshwater	pipelines	flexibility index	freshwater usage (ton/h)
1	NLP-FI	10%	20%	**1.894**	**440**
2	NLP-SC	**5.04%**	20%	1	**420.17**

Table 3. Nominal Stream Data of Water Sources in Example 2

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

written as

$$f_p^{in} = f_p^{out} \quad p \in \mathbb{P}_2 \tag{21}$$

Notice that this assumption can be easily relaxed and the generalized model formulation can be found elsewhere.[3]

On the other hand, since only the mass balance of one key contaminant is considered in this work, the corresponding constraint should be

$$f_p^{in} c_p^{in} = \sum_{p' \in \mathbb{P}_2} f_{p',p} c_{p'}^{out} + \sum_{w \in \tilde{\mathbb{W}}} f_{w,p}^{W} \overline{C}_w \theta_w^{W} \quad p \in \mathbb{P}_2 \tag{22}$$

where, c_p^{in} and $c_{p'}^{out}$ denote the concentrations at the inlet of unit p and outlet of unit p' respectively; $\overline{C}_w$ denotes the nominal concentration from water source w and θ_w^W is the corresponding uncertain multiplier.

The upper bounds of key contaminant concentrations at the mixing nodes before all water using and wastewater treatment units:

$$c_p^{in} \le \overline{C}_p^{in} \theta_p^{in} \quad p \in \mathbb{U} \cup \mathbb{T} \tag{23}$$

where, $\overline{C}_p^{in}$ is the nominal value of maximum allowable concentration at the mixing node before unit p, and θ_p^{in} is the corresponding uncertain multiplier.

1. **Water using units.** The process performance of a water using unit can be characterized as

$$f_u^{in} c_u^{in} + \theta_u^M \overline{M}_u = f_u^{out} c_u^{out} \quad u \in \mathbb{U} \tag{24}$$

where c_u^{in} and c_u^{out}, respectively, represent the inlet and outlet concentrations of water using unit u; $\overline{M}_u$ denotes the nominal mass load of unit u and θ_u^M is the corresponding uncertain multiplier.

The maximum outlet concentration limits of water using units is as follows:

$$c_u^{out} \le \overline{C}_u^{out} \theta_u^{out} \quad u \in \mathbb{U} \tag{25}$$

where $\overline{C}_u^{out}$ represents the nominal value of maximum allowable outlet concentration for unit u, while θ_u^{out} is the corresponding uncertain multiplier.

2. **Wastewater treatment units.** For each wastewater-treatment unit, the performance equation is

$$c_t^{out} = c_t^{in}(1 - \theta_t^R \overline{R}_t) \quad t \in \mathbb{T} \tag{26}$$

where, c_t^{in} and c_t^{out} represent the inlet and outlet concentrations of wastewater treatment unit t respectively; $\overline{R}_t$ denotes the nominal value of removal ratio of unit t and θ_t^R is the corresponding uncertain multiplier.

The maximum throughput limits of wastewater treatment units:

$$f_t^{in} \le F_t \quad t \in \mathbb{T} \tag{27}$$

where F_t represents the specified maximum throughput of unit t. It should be noted that the flexibility index model is supposed to be applied to a given (or existing) water network and the processing capacity of every treatment unit should be fixed in this design. Consequently, the maximum treatment throughputs are not regarded as uncertain parameters in this work.

3. **Mixers.** For any mixer, the corresponding performance equation can simply be written as

$$c_a^{in} = c_a^{out} \quad a \in \mathbb{A} \tag{28}$$

where, c_a^{in} and c_a^{out} are the inlet and outlet concentrations, respectively, of mixer a.

4.2.3. Sinks. At the mixing node of each sink d, the flow and contaminant balances are

$$f_d^{in} = \sum_{p \in \mathbb{P}_2} f_{p,d}^{D} + \sum_{w \in \mathbb{W}} f_{w,d}^{W} \quad d \in \mathbb{D} \tag{29}$$

$$f_d^{in} c_d^{in} = \sum_{p \in \mathbb{P}_2} f_{p,d}^{D} c_p^{out} + \sum_{w \in \mathbb{W}} f_{w,d}^{W} \overline{C}_w \theta_w^{W} \quad d \in \mathbb{D} \tag{30}$$

where f_d^D is the total water flow rate after the mixing node of sink d; c_d^{in} is the corresponding concentration; $\overline{C}_w$ is the nominal value

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Table 4. Nominal Design Specifications of Water Using Units in Example 2

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

Table 5. Nominal Design Specifications of Wastewater Treatment Units in Example 2

unit	$\overline{C}^{in}_{max}$ (ppm)	$\overline{F}^{in}_{max}$ (ton/h)	removal ratio ($\overline{R}$)
t1	185	125	0.9
t2	200	135	0.8

of the concentration at source w and θ^W_w is the corresponding uncertain multiplier.

The upper bounds of contaminant concentrations at the mixing nodes before all sinks is

$$c^{in}_d \leq \overline{C}^{in}_d \quad d \in \mathbb{D} \tag{31}$$

where, $\overline{C}^{in}_d$ is the nominal value of maximum allowable concentration at the mixing node before unit d. Note that, since this inequality constraint is imposed mainly to comply with environmental regulations, the upper bound of c^{in}_d is regarded as a constant in the present study.

Finally, it should be noted that some of the aforementioned constraints, that is, eqs 22, 24 and 30, are bilinear and thus the proposed models must be nonconvex. Although in principle global optima cannot always be guaranteed, the reliable GAMS module BARON[16] has been adopted in this work to solve every problem repeatedly so as to ensure satisfactory convergence.

4.3. Additional Constraints. Other than the aforementioned constraints traditionally included in the mathematical model for water-network design, additional ones are needed in the improved flexibility index model and they are listed in the sequel:

1. **Overdesign levels.** The larger-than-normal design specifications considered in this work are concerned with flow capacities exclusively. Specifically, the overdesign level of the freshwater supply system can be expressed as

$$\mathrm{sr}_w \leq S^{(1)}_w(1 + O_w) \quad w \in \mathbb{W}_1 \tag{32}$$

where, $S^{(1)}_w$ and O_w respectively represent the nominal supply rate and the corresponding overdesign percentage of freshwater w, and they should be considered as given parameters.

On the other hand, the upper limit of flow rate in each existing pipeline can be written as

$$f_{p,p'} \leq F_{p,p'}\left(1 + O_{p,p'}\right) \quad p, p' \in \mathbb{P}_2 \tag{33}$$

$$f_{p,d} \leq F_{p,d}\left(1 + O_{p,d}\right) \quad p \in \mathbb{P}_2 \quad d \in \mathbb{D} \tag{34}$$

$$f_{w,p} \leq F_{w,p}\left(1 + O_{w,p}\right) \quad w \in \mathbb{W} \quad p \in \mathbb{P}_2 \tag{35}$$

where, $F_{p,p'}$, $F_{p,d}$ and $F_{w,p}$ are normal flow rates of the existing streams associated respectively with $f_{p,p'}$, $f_{p,d}$ and $f_{w,p}$, while $O_{p,p'}$, $O_{p,d}$, and $O_{w,p}$ are the corresponding overdesign levels.

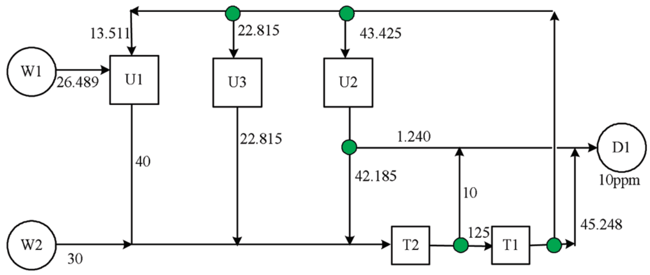

Figure 5. Design I in example 2.

2. **Critical direction.** According to the observations given in section 3, the critical direction in eq 6 can be defined more explicitly as

$$\theta^W_w = 1 + \delta\Delta\theta^{W+}_w, \quad w \in \mathbb{W} \tag{36}$$

$$\theta^{in}_p = 1 - \delta\Delta\theta^{in-}_p, \quad p \in \mathbb{P}_1 \tag{37}$$

$$\theta^{out}_u = 1 - \delta\Delta\theta^{out-}_u, \ \theta^M_u = 1 + \delta\Delta\theta^{M+}_u, \quad u \in \mathbb{U} \tag{38}$$

$$\theta^R_t = 1 - \delta\Delta\theta^{R-}_t, \quad t \in \mathbb{T} \tag{39}$$

where δ is a nonnegative scalar variable; $\Delta\theta^{W+}_w$ and $\Delta\theta^{M+}_u$, respectively, denote the expected positive deviations of the pollutant concentration of water source w and the mass load of water using unit u; $\Delta\theta^{in-}_p$, $\Delta\theta^{out-}_u$, and $\Delta\theta^{R-}_t$, respectively, represent the expected negative deviations of the maximum allowable inlet concentration of unit p, the maximum allowable outlet concentration of water using unit u, and the removal ratio of treatment unit t.

On the basis of the aforementioned definition, the validity of the proposed approach can be argued as follows. First of all, it should be noted that the optimal solution of the original flexibility index model must also be a feasible solution of the NLP-FI model. This is true because the constraints given in eq 6 are just a subset of those in eq 3. Second, it can be observed that eqs 36−39 represent the most constrained direction away from the nominal point in the uncertain parameter space. More specifically, if the NLP-FI model is solved along the critical direction, the resulting flexibility index (denoted as δ^*) should in general be smaller than that obtained in any other direction. For example, if the proposed critical direction is altered by replacing eq 36 with $\theta^W_w = 1 + \delta\Delta\tilde{\theta}^{W+}_w$ and $\Delta\tilde{\theta}^{W+}_w < \Delta\theta^{W+}_w$, then the inlet and outlet concentrations of its downstream water-using units and wastewater treatment units should all be driven to lower levels at $\delta = \delta^*$. As a result, a higher operational flexibility can be obtained by searching in this altered direction. Since it is clear that the same arguments can be made concerning the other uncertain parameters, one can safely conclude that the flexibility index can almost always be obtained by solving the proposed NLP-FI model.

3. **Nonexistent flows.** 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

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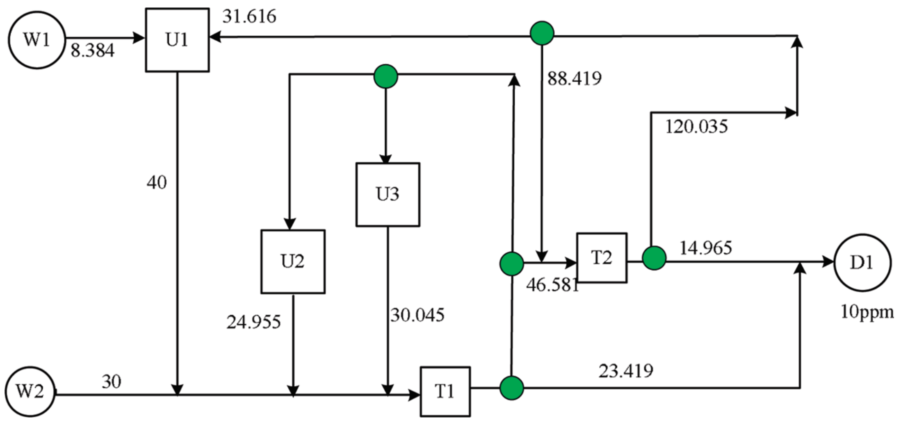

Figure 6. Design II in example 2.

Table 6. Nominal Operating Conditions of All Units in Design I for Example 2

unit	u1	u2	u3	t1	t2	d1
flow rate (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 7. Nominal Operating Conditions of All Units in Design II for Example 2

unit	u1	u2	u3	t1	t2	d1
flow rate (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	

constraints. For illustration convenience, let us define the set of all branches in a superstructure as follows:

$$\mathbb{L} = \{l | l \text{ is the label of a branch in the superstructure}\}$$

where $\mathbb{L} = \mathbb{L}_0 \cup \mathbb{L}_1$ and

$$\mathbb{L}_0 = \{l_0 | l_0 \text{ is the label corresponding to a nonexistent branch in the given network}\}$$

$$\mathbb{L}_1 = \{l_1 | l_1 \text{ is the label corresponding to an existing branch in the given network}\}$$

Thus, a general form of constraints on the flow rates of nonexistent branches used in a particular application should be written as

$$f_l = 0 \quad l \in \mathbb{L}_0 \tag{40}$$

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

5. ALTERNATIVE FLEXIBILITY ASSESSMENT MODELS

The aforementioned model can be modified slightly to perform other important tasks for flexibility assessment. Under the condition that the given nominal network is infeasible, these modified versions can be used to determine the exact (lowest) overdesign level of freshwater supply system and/or to identify the optimal structural changes so as to cope with all possible variations defined in the *expected* region of uncertain parameters, that is, when $\delta = 1$ in eq 3. Their formulations are summarized in the sequel as follows.

Table 8. Comparison of Main Results Based on Design I in Example 2

step	model	overdesign: freshwater	overdesign: pipelines	flexibility index	freshwater usage (ton/h)
1	NLP-FI	30%	50%	**0.765**	**26.489**
2	NLP-FI	relaxed	50%	**1.351**	**39.734**
2	NLP-SC	**38.25%**	50%	1	**36.62**

Table 9. Critical Operating Conditions of All Units in Design II-A for Example 2

unit	u1	u2	u3	t1	t2	d1
flow rate (ton/h)	42.007	26.758	26.234	125.000	135.000	72.007
c^{in} (ppm)	0.100	18.241	18.241	164.724	5.561	10.000
c^{out} (ppm)	101.000	240.000	200.000	18.241	1.165	

5.1. Minimal Source Capacity. The modified model for calculating the smallest upper limit of total freshwater supply rate is referred to as the NLP-SC model. The model formulation can be expressed as

$$\min \sum_{w \in \mathbb{W}_1} sr_w$$

subject to equations 16−40, and

$$\delta = 1 \tag{41}$$

Notice that, since usually there is only one primary source, the minimized objective value in this case can also be used to determine the desired overdesign level of the freshwater supply system.

5.2. Optimal Network Reconfiguration. In this work, the network configuration is modified by adding new pipelines and/or removing existing ones. In principle, these pipelines are selected mainly to relax one or more active constraints[6] so as to create chances for further flexibility increase. This point will be elaborated later in case studies. To facilitate construction of a mathematical programming model to automatically revise the

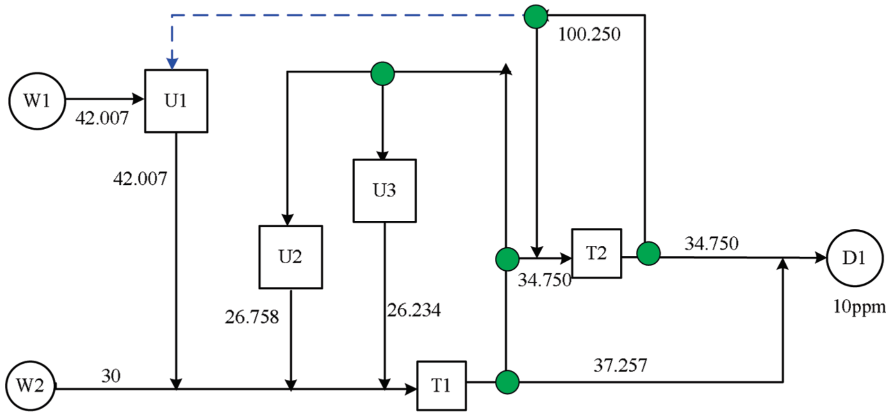

Figure 7. Critical operating conditions of Design II-A in example 2.

network connections, the following binary variables must be used

$$f_{p,p'} \leq n_{p,p'}\mathrm{FU} \quad p, p' \in \mathbb{P}_2 \tag{42}$$

$$f_{p,d} \leq n_{p,d}\mathrm{FU} \quad p \in \mathbb{P}_2 \quad d \in \mathbb{D} \tag{43}$$

$$f_{w,p} \leq n_{w,p}\mathrm{FU} \quad w \in \mathbb{W} \quad p \in \mathbb{P}_2 \tag{44}$$

where FU is a large enough positive number; $n_{p,p'}$, $n_{p,d}$, and $n_{w,p}$ are the binary variables used to signify whether or not the *selected* pipelines exist in the final network configuration.

To minimize the total capital expenditure, the following simple objective function is used in the new MINLP model:

$$\min[\Phi_{\mathrm{pl}}(\sum_{p,p' \in \mathbb{P}_2} n_{p,p'} + \sum_{p \in \mathbb{P}_2, d \in \mathbb{D}} n_{p,d} + \sum_{w \in \mathbb{W}, p \in \mathbb{P}_2} n_{w,p}) + \sum_{w \in \mathbb{W}_1} \Phi_w \mathrm{sr}_w] \tag{45}$$

where Φ_{pl} is the average annual cost for installing and operating a pipeline and Φ_w is the unit annual cost of freshwater supply system w. It should be noted that more elaborate cost model can certainly be adopted if accurate cost data are available. Notice also that the model constraints in this mathematical program have already been described in equations 16−44, and it is referred to as the MINLP-NR model in the present paper.

6. CASE STUDIES

Two case studies are presented below to demonstrate the usefulness of the proposed models. Uncertain upper limits of the inlet and outlet concentrations of the water using units are considered in the first example, while the uncertainties embedded in the contaminant concentration in the secondary water, the mass loads of water using units and the removal ratios of treatment units are studied in the second example.

All models were solved with GAMS modules (version 22.4)[16] on a PC with an Intel(R) Core(TM) CPU at 2.66 GHz. Although the default NLP solver in GAMS is CONOPT3 and MIP solver is CPLEX, BARON is adopted to solve both NLP and MINLP models.[15] In addition, since the starting point of optimization computation usually exerts a profound influence on the convergence process of MINLP models, a reliable initialization procedure was developed to promote convergence.[4] For the sake of completeness, a concise version of this procedure is given in the Supporting Information.

6.1. Example 1.

Let us first consider an existing water network (see Figure 3), which consists of a single water source and two water-using units, and those numbers in parentheses are concentrations. The design specifications of the water-using units are provided in Table 1. The contaminant concentration in freshwater is 20 ppm. It is assumed that the maximum inlet and outlet contaminant concentrations of unit 1, C_1^{in} and C_1^{out}, and the maximum contaminant concentration at the outlet of unit 2, C_2^{out}, vary with the ambient temperature. A typical example of this phenomenon is the desalter in petroleum processing, in which the salt solubility varies with water 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 $\theta_1^N = \theta_2^N = \theta_3^N = 1$, and two splitters are marked by small circles in Figure 3. The split ratios of their two branch streams can be adjusted to compensate external disturbances during operation. In addition, let us assume that the overdesign levels of the freshwater supply system and all pipelines are set at 10% and 20%, respectively.

According to the assessment procedure described in Figure 1, the proposed flexibility index model NLP-FI should be applied first. There are a total of 10 variables in this model, and the corresponding flexibility index was easily determined to be 1.894 by the BARON solver. The obtained critical solution can be found in Figure 4. Since the flexibility index of the given design is much larger than 1, the proposed NLP-SC model can be used to find the minimum overdesign level of freshwater supply system. The total number of variables is reduced to be 9 in the NLP-SC model because the flexibility index has been fixed to be 1 according to eq 41. In the optimization results, it was found that the corresponding upper limit of freshwater usage should be 420.17 ton/h with an overdesign percentage of 5.04%. It should be noted that above optimization computations all converged within 0.1 s, while the same results were obtained in Chang et al.[4] with a much longer solution time (1 s). Other means of flexibility improvement, such as adding or removing pipelines, are not considered here because the present one is already flexible enough. Finally, for comparison convenience, the main results obtained in this example are summarized in Table 2. Notice that the boldfaced values can be identified from optimal solutions.

6.2. Example 2. Let us next consider a grass-root design problem.[4] Specifically, there are two water sources, three water-using units, two wastewater treatment units, and a wastewater sink in the chemical process under consideration. The nominal flow rate ($\bar{F}^{W}$) and contaminant concentration ($\bar{C}^{W}$) of the water sources, that is, freshwater w1 and secondary water w2, are provided in Table 3. The design specifications of water using units and wastewater treatment units under nominal conditions are provided in Table 4 and Table 5, respectively. Finally, the pollutant concentration at the sink is required to be kept below 10 ppm.

By minimizing the freshwater consumption rate on the basis of superstructures, two alternative designs were generated with the aforementioned nominal data (see Figures 5 and 6).[4] For convenience, they are referred to as Design I and Design II, respectively. The corresponding operating conditions of the water using and wastewater treatment units are provided in Tables 6 and 7. In this example, these two network structures are used as the base-case designs for the subsequent flexibility analysis. Notice that, although the numbers of branch streams (12) and splitters (5) are the same in both networks, the freshwater usage of Design I is 26.489 ton/h, while much less (8.384 ton/h) is needed in Design II. The reduction of freshwater requirement is achieved in the latter case by allowing the self-recycle stream around treatment unit t2. The overdesign levels of freshwater supply system and all pipelines in both designs are set at 30% and 50%, respectively. Therefore, the upper bound of freshwater consumption rate should be 34.436 ton/h in Design I, while it is 10.90 ton/h in Design II.

Let us assume in this example that the external disturbances during normal operation may cause three types of design parameters fluctuate: (1) the contaminant concentration in secondary water, (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 generalized flexibility index model:

$$0.9 \le \theta_2^{W} \le 1.1$$

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

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

Notice that these multipliers have been defined in eqs 22, 24, and 26, respectively.

The proposed flexibility assessment procedure (see Figure 1) can be applied to the two nominal designs mentioned above. A brief summary of the implementation steps is given below:

(1) It should be first noted that about 69 variables and 41 constraints are involved in the NLP-FI and NLP-SC models for both nominal designs in this example. The flexibility indices of Design I and Design II can be found with the NLP-FI model to be 0.765 and 0.113, respectively. In both cases, the freshwater consumption rates at critical conditions reached their respective upper bounds. Thus, it is clear that the expected uncertain disturbances cannot be compensated by adjusting the control variables in both cases. The subsequent assessment steps should then be applied to these two nominal designs individually.

(2) Assessment results for Design I: The possibility of raising the operational flexibility of Design I by relaxing the upper bound of freshwater supply rate is first explored. It was found by solving the NLP-FI model again that the flexibility index can be improved to 1.351 if this upper limit is increased to 40 ton/h. Under the critical condition, the freshwater consumption rate was 39.734 ton/h since the upper limit of one or more pipeline capacity was reached. The corresponding minimum upper limit of the freshwater supply rate was then determined to be 36.62 ton/h with the proposed NLP-SC model. This result is the same as that reported in Chang et al.[4] Thus, the overdesign level of the freshwater supply system in Design I should be at least be 38.25%. Finally, note that a summary of the above assessment findings is also presented in Table 8.

(3) Assessment results for Design II:

(a) The upper limit of freshwater supply rate was first raised to 20 ton/h. By solving the NLP-FI model, the flexibility index became 0.190 in this case. The reason

Table 10. Critical Operating Conditions of All Units in Design II-B for Example 2

unit	u1	u2	u3	t1	t2	d1
flow rate (ton/h)	66.652	42.631	36.541	125.000	135.000	80
c^{in} (ppm)	1.000	80	50	185.00	15.762	10.000
c^{out} (ppm)	74.097	240.000	200.000	25.760	3.702	

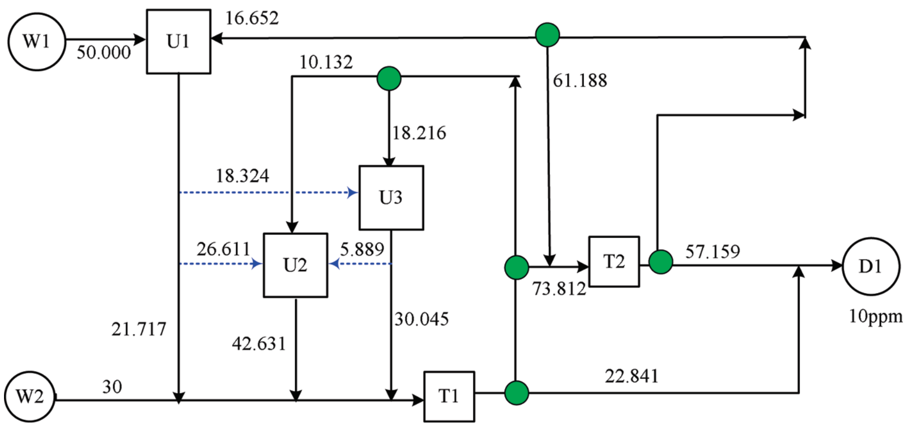

Figure 8. Critical operating conditions of Design II-B in example 2.

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for such small improvement is that the critical freshwater usage is 12.576 ton/h, which is the result of one or more upper limit imposed upon pipeline capacity. Next, the model constraints were further relaxed by removing all capacity limits on the water flows in existing pipelines, and the upper limit of freshwater supply rate was increased to 50 ton/h (denoted as Design II-A). The resulting flexibility index was also computed with the NLP-FI model, and this value is 0.398. The obtained critical conditions are presented in Table 9 and Figure 7. Note that the dash line in Figure 7 means that there is no flow under the critical condition. These results also show that raising the freshwater capacity to any level higher than the critical value (42.01 ton/h) is useless.

(b) It can be observed from Table 9 that the upper limits of c_{d1}^{in}, c_{u1}^{out}, c_{u2}^{out}, c_{u3}^{out}, f_{t1}^{in}, and f_{t2}^{in} are reached, and thus the corresponding inequalities are the active constraints[6] in Design II-A. Obviously, the flexibility index can be increased only if the active constraints are relaxed. Thus, new auxiliary pipelines may be added so as to facilitate relaxation of such constraints.[5] Since it is clearly not feasible to lower the throughput of any wastewater treatment unit by feeding an extra water flow to its inlet, only the possibilities of relaxing the first four inequality constraints are considered here. These considerations are summarized as follows:
(i) Since sink d1 already accepts water streams from t1 and t2 in the present network, it is only necessary to consider other sources. Notice that the concentration at the sink c_{d1}^{in} is less likely be lowered by adding a pipeline from any of the water using units, that is, u1, u2, or u3 to sink d1. This is because the outlet concentrations of these units all reach their maxima in the optimal solution, which is much larger than the allowed maximum value of c_{d1}^{in}. It should also be noted that dilution of effluent to sink d1 directly with freshwater w1 is not allowed in the present study. Therefore, it can be concluded that the active constraint corresponding to c_{d1}^{in} cannot be relaxed by introducing new pipelines. (ii) The option of adding an extra water flow to lower c_{u1}^{out} should be ignored because unit u1 has the lowest concentration limits both on its inlet and outlet. (iii) Based on the optimal conditions of water utilization system,[17] the used water from u1 can be partly reused in u2 to reduce c_{u2}^{out}. This mainly is because the allowed maximum outlet concentration of u1 is much less than that of u2, and also there is still room for the inlet concentration of u2 to increase. (iv) For the same reason, pipelines from u1 to u3 and from u3 to u2 may be added to Design II-A.
The revised network is referred to as Design II-B and the corresponding flexibility index found by solving the NLP-FI model is 1.4535. The resulting critical operating conditions are given in Table 10 and Figure 8. Notice that the added auxiliary pipelines are marked with blue dotted lines.

(c) Design II-B was then reconfigured with the MINLP-NR model. By setting the cost coefficients Φ_{pl} and Φ_w to be 1 and 0.5, respectively, Design II-C can be obtained. The optimal solution is shown in Table 11 and Figure 9. In this case, the minimum total annual cost is 26.840 and the freshwater consumption rate is 27.680 ton/h. Notice that one of the added pipelines is eliminated in the optimal network (as shown with a blue dash line) while one existing branch is also removed (as shown with a black dash line). It should also be noted that a total of 82 constraints, 84 continuous variables, and 26 binary variables are involved in this MINLP-NR model.

(d) It should be noted that the optimal solution is not unique. Other alternatives can be easily created by slightly changing the initial guess or using a different solver. An example is given in Figure 10 (Design II-D). While the objective value of this design is the same as that of Figure 9, only one of the three added auxiliary pipelines is kept in this solution.

A summary of the assessment results for Design II can be found in Table 12. It should be noted that all aforementioned models converged within 2 s of CPU time, except that about 18 s of CPU

Table 11. Critical Operating Conditions of All Units in Design II-C for Example 2

Unit	u1	u2	u3	t1	t2	d1
flow rate (ton/h)	46.000	61.240	33.760	125.000	135.000	57.680
c^{in} (ppm)	1.000	68.261	46.712	178.578	10.535	10.000
c^{out} (ppm)	101.000	173.421	200.000	22.679	2.360	

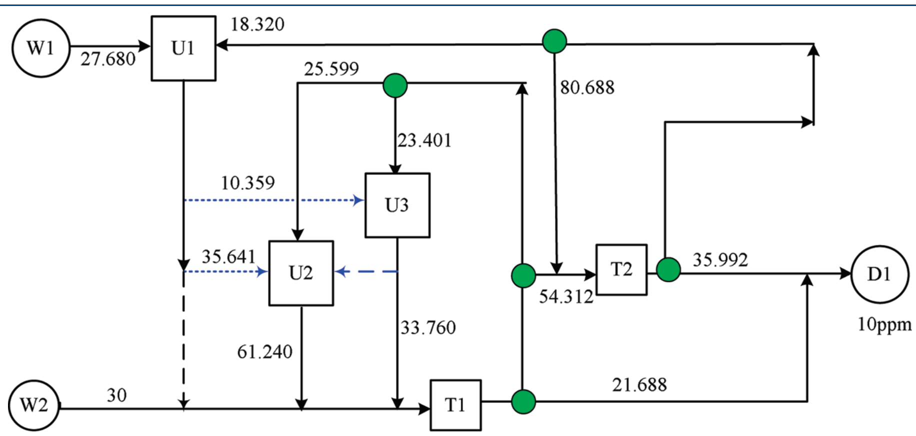

Figure 9. Critical operating conditions of Design II-C in example 2.

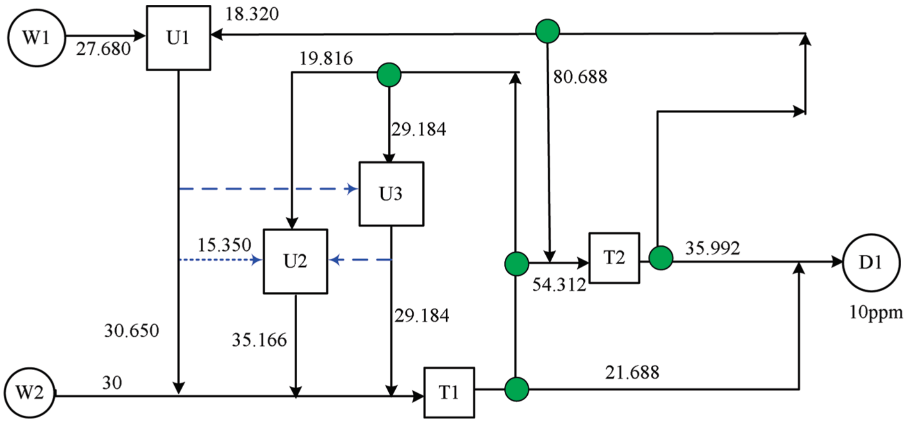

Figure 10. Alternative operating conditions of Design II-D in example 2.

Table 12. Comparison of Main Results Based on Design II in Example 2

step	model	overdesign freshwater	overdesign pipelines	flexibility index	freshwater usage (ton/h)	renamed as
1	NLP-FI	30%	50%	**0.113**	**8.384**	
2	NLP-FI	relaxed	50%	**0.190**	**12.576**	
3	NLP-FI	relaxed	relaxed	**0.389**	**42.07**	Design II-A
4	NLP-FI	relaxed	relaxed	**1.4535**	**50**	Design II−B
5a	MINLP-NR	relaxed	relaxed	1	**27.681**	Design II−C
5b	MINLP-NR	relaxed	relaxed	1	**27.681**	Design II-D

time is needed for the MINLP-NR models of Design II-D, which are much shorter than the reported values, that is, within 100 s.[4]

7. Conclusions. A mathematical programming approach is proposed in this paper to assess the operational flexibility of given water networks. The flexibility of a given water network can be improved by relaxing the upper limit of freshwater supply rate and/or incorporating structural modifications. It has been shown in the case studies that the proposed assessment procedure is feasible and efficient. Furthermore, the following conclusions can also be drawn from the optimization results obtained in the examples: (1) The proposed NLP-FI model is much easier to solve than the existing active-constraint based formulation, while the same quality solutions can be obtained in both cases; (2) The traditional ad hoc approach to set the overdesign levels on freshwater supply system and pipelines may not be sufficient to overcome all uncertain disturbances. The proposed NLP-SC model represents a better alternative which could be used to exactly determine the minimum freshwater supply capacity; (3) The proposed MINLP-NR model can be used to automatically add/remove pipelines so as to achieve a desired level of operational flexibility.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information. The initialization procedure for the proposed models. This material is available free of charge via the Internet at http://pubs.acs.org.

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■ NOMENCLATURE

Sets, Parameters, and Variables

δ = variable of flexibility index
θ = set of uncertain parameters
Θ = parameter space of θ
$\mathbb{A}$ = set of mixer units
C, c = concentration
d = vector of design variables
$\mathbb{D}$ = set of water sinks
f = flow rate
FU = a big enough positive number
g = vector of inequality constraints
h = vector of equality constraint
$\mathbb{I}$ = index set of equality constraint
$\mathbb{J}$ = index set of of inequality constraint
$\mathbb{L}$ = set of branches in the superstructure
M = mass load of water-using unit
n = binary variable
$\mathbb{P}_1$ = union set of $\mathbb{U}$ and $\mathbb{A}$
$\mathbb{P}_2$ = union set of $\mathbb{U}$, $\mathbb{T}$ and $\mathbb{A}$
$\mathbb{T}$ = set of wastewater treatment units
$\mathbb{U}$ = set of water-using units
$\mathbb{W}$ = set of water sources
x = vector of state variables
z = vector of control variables

Superscripts

+ = positive
D = wastewater sink
M = mass load
out = outlet
W = water source
− = negative
in = inlet
N = nominal
R = removal ratio

Subscripts

a = mixer
i = equality constraint
p, p' = process unit in $\mathbb{P}$
u = water-using unit
d = water sink
j = inequality constraint
t = treatment unit
w = water source

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