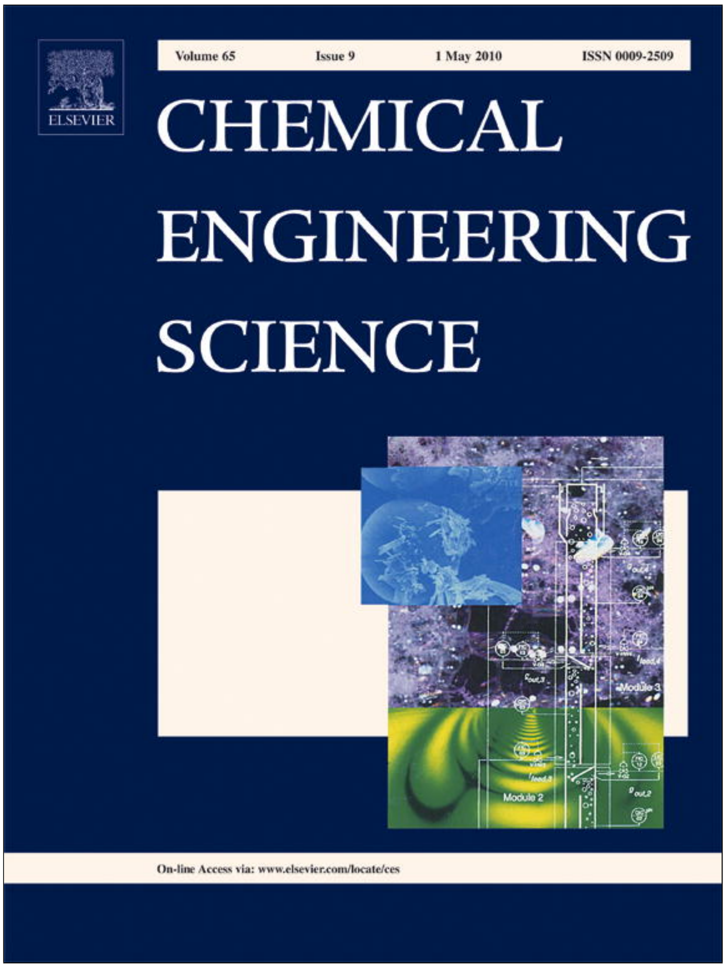
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A heuristic revamp strategy to improve operational flexibility of water networks based on active constraints

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ABSTRACT

A novel heuristic revamp strategy is presented in this paper to improve the operational flexibility of existing water networks. The well-established concept of *flexibility index* (Swaney and Grossmann, 1985a, b) is adopted for quantitatively characterizing the ability of a given water network to cope with uncertain disturbances. Since it is necessary to solve a mixed-integer nonlinear program (MINLP) for this purpose, the convergence of corresponding numerical optimization process is not guaranteed. Two solution techniques are developed to promote efficiency, namely (1) generating the initial guesses by minimizing freshwater consumption rate of the nominal network structure, and (2) incorporating the smoothing functions to eliminate the binary variables in the MINLP model. A set of heuristics are also suggested to identify possible measures for relaxing the active constraints in the resulting optimal solution. Other than increasing the upper limit of freshwater supply rate, additional flexibility enhancement options concerning structural changes (which have never been systematically applied before) are considered thoroughly in the present study. These revamp methods include: (1) inserting/deleting pipeline connections and (2) adding/replacing treatment units. The implementation results of several case studies are provided at the end of this paper to demonstrate the effectiveness of proposed strategy.

1. Introduction

Water is an essential natural resource needed in almost every process plant. For instance, it is used for crude oil desalting in the petroleum refineries, for liquid–liquid extraction in hydrometallurgical processes, for cooling, quenching and scrubbing in the iron and steel industry, and for various washing operations in the food processing facilities. Due to the bleak forecast concerning water shortage in the next decade and also the increasingly stringent environmental regulations for wastewater disposal, efficient water utilization is obviously an indispensable criterion that must be adopted for designing any industrial process (Dudley, 2003).

Various industrial water management issues have already been addressed extensively in the literature. In particular, a number of mathematical programming models were developed to optimally route the process streams in a water network for the purpose of minimizing freshwater consumption rate and/or wastewater generation rate. One of the pioneering papers in this area was published by Takama et al. (1980), who studied the optimal water allocation problem in a petroleum refinery. Wang and Smith (1994) suggested to consider water reuse, regeneration–reuse and regeneration–recycling in water network designs as viable wastewater minimization strategies. They also proposed a heuristical methodology for designing effluent treatment systems in which wastewaters were processed in a distributed manner. Alva-Argaez et al. (1998) used a mathematical programming approach to optimize a superstructure in which all possibilities of water treatment and reuse were embedded. Bagajewicz et al. (1999) developed a systematic method to transform the nonlinear model for multi-contaminant large-scale water system designs to a linear program (LP). Another important work was carried out by Huang et al. (1999), who presented a comprehensive programming approach to synthesize the optimal water usage and treatment networks in chemical processes. Feng and Seider (2001) assessed the feasibility of simplifying the network configurations in large plants with internal water mains. Karrupiah and Grossmann (2006) studied the optimal synthesis problem of integrated water systems, where water using and treatment operations were incorporated into a single network in such a way that the total annual cost could be minimized.

From the above studies, it can be observed that complex configurations are often needed in the optimal water networks to facilitate extensive reuse–recycle and reuse–regeneration. These structures obviously hamper efficient operation and control under uncertain disturbances from environment. In the past, very few studies have been performed to deal with this important issue. Tan and Cruz (2004) formulated two different versions of the *symmetry fuzzy linear programming* (SFLP) models for the purpose

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of synthesizing robust water-reuse networks based on imprecise process data. Al-Redhwan et al. (2005) developed a three-step procedure to design water networks under uncertain operating temperatures and pressures. Tan et al. (2007) used the Monte Carlo simulation techniques to analyze the vulnerability of water networks with noisy mass loads. Karrupiah and Grossmann (2008) proposed a spatial branch-and-cut algorithm to locate the global optimum. Zhang et al. (2009) suggested to use the concepts 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. The latest contribution was published by Li et al. (2009). A generalized mathematical programming model was adopted as the design tool for improving the operational flexibility of any given network with two specific revamp options, i.e., (1) relaxation of the upper limit of freshwater supply rate and (2) installation of auxiliary pipelines and/or elimination of existing ones. Although this strategy was successfully implemented with an ad hoc approach in various applications, there are still incentives to develop a structured procedure so as to generate satisfactory designs more consistently. Furthermore, a third flexibility enhancement measure was often ignored in the previous studies, i.e., upgrading the existing wastewater treatment units and/or placing new ones. It is therefore necessary to integrate this additional option into the aforementioned revamp procedure as well.

The flexibility index is a well-established concept for quantitatively characterizing the ability of an existing process to cope with uncertain disturbances (Swaney and Grossmann, 1985a, b). Grossmann and Floudas (1987) have formulated a mixed-integer nonlinear programming model accordingly and then solved the model with the so-called active constraint strategy. A modified version of this general model, in which the constraints are taken from Huang et al. (1999), is used in the present work for evaluating the flexibility level of any given water network. To facilitate efficient solution, Bandoni et al. (2000) suggested that the binary variables in the MINLP formulation can be removed with smoothing functions. This approach and the specific smoothing function proposed by Biegler and Balakrishna (1992) are adopted to reformulate the original flexibility index model as a simpler nonlinear program to produce approximate solutions which may not be globally optimal. On the other hand, an effective initialization strategy has also been developed for the original MINLP model. In particular, an alternative optimization problem is solved by minimizing the freshwater consumption rate of the nominal network. The optimization results of this problem can then be used as the initial guesses for computing the flexibility index. A set of heuristics have been developed to identify possible revamp measures for relaxing the active constraints in the optimal solution of flexibility index model. Other than increasing the upper limit of freshwater supply rate, two structural modifications are considered as the main revamp options, i.e., (1) inserting/deleting pipeline connections and (2) adding/replacing treatment units. The proposed revamp procedure has been tested in several case studies.

The remaining part of this paper is organized as follows. The flexibility assessment procedure is first given in Section 2. Next the solution strategies of the flexibility index model are elaborated in Section 3. The systematic procedure to improve the flexibility level of a water network is then explained in Section 4. Section 5 contains the case studies for testing the proposed flexibility enhancement procedure. Finally the conclusions are outlined in the last section.

2. Flexibility assessment method for water networks

Since it is very tedious and inefficient to construct different versions of the flexibility index model for various candidate network configurations obtained in revamp studies and then carry out the needed optimization computations, a generalized model formulation is used in this work for all possible alternative structures.

2.1. Superstructure

To facilitate a concise description of the superstructure for incorporating all possible network configurations and also the corresponding mathematical models, let us define the label sets for the water sources, water-using unit, water treatment units and sinks as follows:

$$\mathbb{W}_1 = \{w_1 | w_1 \text{ is the label of a primary water source}\} \tag{1}$$

$$\mathbb{W}_2 = \{w_2 | w_2 \text{ is the label of a secondary water source}\} \tag{2}$$

$$\mathbb{S} = \{s | s \text{ is the label of a sink}\} \tag{3}$$

$$\mathbb{U} = \{u | u \text{ is the label of a water using unit}\} \tag{4}$$

$$\mathbb{T} = \{t | t \text{ is the label of a water treatment unit}\} \tag{5}$$

Let us further denote the sets of all sources and all processing units respectively as

$$\mathbb{W} = \mathbb{W}_1 \cup \mathbb{W}_2 \tag{6}$$

$$\mathbb{P} = \mathbb{U} \cup \mathbb{T} \tag{7}$$

The following steps can be carried out to build the superstructure:

1. Connect every primary water source in $\mathbb{W}_1$ to the inlet of every unit in $\mathbb{P}$.
2. Connect every secondary water source in $\mathbb{W}_2$ to the inlet of every unit in $\mathbb{P}$ and every sink in $\mathbb{S}$.
3. Connect the outlet of every unit in $\mathbb{P}$ to the inlet of every unit in $\mathbb{P}$ and every sink in $\mathbb{S}$.

Since all possible water pathways are embedded in the superstructure, a general design model can be formulated accordingly.

2.2. General design model

To facilitate flexibility assessment, the material-balance constraints must first be established for all components in the water network. These constraints are briefly summarized in the sequel.

2.2.1. Primary sources

The freshwater supplies secured by a chemical plant are usually regarded as the primary water sources in the model. It is also assumed that any effluent is not allowed to be mixed with freshwater to meet the discharge limit required by environmental regulation. Hence the distribution of freshwater in the water network can be described with the following equation:

$$F_{w_1} = \sum_{p \in \mathbb{P}} f_{w_1,p}, \quad w_1 \in \mathbb{W}_1 \tag{8}$$

where F_{w_1} denotes the freshwater supply rate from source w_1, and $f_{w_1,p}$ denotes the flow rate of freshwater from source w_1 to unit p. The freshwater supply rate should of course not exceed a maximum allowable value and thus can be expressed as an inequality constraint, i.e.,

$$F_{w_1} \le F_{w_1}^U, \quad w_1 \in \mathbb{W}_1 \tag{9}$$

where $F_{w_1}^U$ is a *given* upper bound of the freshwater supply rate obtained from source w_1.

2.2.2. Secondary sources

Any secondary water source generally has a higher pollutant concentration than that of every primary source, as it may has already been used by other water system in another plant. The secondary waters can be sent directly to the sinks and their total supply rates and contaminant concentrations are assumed to be fixed at nominal levels. The material balance equations at the secondary sources can be written as:

$$F_{w_2} = \sum_{p \in \mathbb{P}} f_{w_2,p} + \sum_{s \in \mathbb{S}} f_{w_2,s}, \quad w_2 \in \mathbb{W}_2 \tag{10}$$

where F_{w_2} denotes a *given* supply rate from secondary source w_2, $f_{w_2,p}$ denotes the water flow rate from source w_2 to unit p, and $f_{w_2,s}$ denotes water flow rate from source w_2 to sink s.

2.2.3. Sinks

The water and component balances for sinks can be described with the following equations:

$$F_s = \sum_{w_2 \in \mathbb{W}_2} f_{w_2,s} + \sum_{p \in \mathbb{P}} f_{p,s}, \quad s \in \mathbb{S} \tag{11}$$

$$F_s C_s = \sum_{w_2 \in \mathbb{W}_2} f_{w_2,s} C_{w_2} + \sum_{p \in \mathbb{P}} f_{p,s} CO_p, \quad s \in \mathbb{S} \tag{12}$$

where F_s denotes the total wastewater discharge rate at sink s, $f_{w_2,s}$ denotes the water flow rate from source w_2 to sink s, $f_{p,s}$ denotes the water flow rate from unit p to sink s, C_{w_2} represents the pollutant concentration at source w_2 (a given parameter), C_s denotes the concentration of key contaminant at sink s, and CO_p denotes key pollutant concentration at the outlet of unit p. Notice that the bilinear terms in the above component balances, i.e., the products of flow rate and concentration are clearly nonconvex.

In addition, an upper concentration limit should be imposed upon every effluent, i.e.,

$$C_s \le C_s^U, \quad s \in \mathbb{S} \tag{13}$$

where C_s^U denotes the maximum pollutant concentration allowed at sink s, which is a given design parameter.

2.2.4. Processing units

Due to the assumption that leaks do not occur in any processing unit, the water throughput of unit p can be computed with two alternative material-balance relations, i.e.,

$$F_p = \sum_{w \in \mathbb{W}} f_{w,p} + \sum_{p' \in \mathbb{P}} f_{p',p} = \sum_{p' \in \mathbb{P}} f_{p,p'} + \sum_{s \in \mathbb{S}} f_{p,s}, \quad p \in \mathbb{P} \tag{14}$$

where F_p denotes the throughput of unit p, $f_{w,p}$ denotes the water flow rate from source w to unit p, $f_{p',p}$ and $f_{p,p'}$ respectively denote the water flow rate from unit p' to unit p and vice versa, and $f_{p,s}$ denotes water flow rate from unit p to sink s. On the other hand, the component balance at the inlet of unit p can be expressed as

$$F_p CI_p = \sum_{w \in \mathbb{W}} f_{w,p} C_w + \sum_{p' \in \mathbb{P}} f_{p',p} CO_{p'}, \quad p \in \mathbb{P} \tag{15}$$

where CI_p denotes the pollutant concentration at the inlet of unit p, C_w denotes the pollutant concentration at source w (which is a given design parameter), and $CO_{p'}$ denotes the pollutant concentration at the outlet of unit p'. Note again that this equation contains bilinear terms. Furthermore, the processing units in a water network can often be divided into two types:

1. *Water-using units*: The conventional mathematical model has been adopted in this study to characterize the water-using operations, i.e.,

   $$F_u(CO_u - CI_u) = M_u, \quad u \in \mathbb{U} \tag{16}$$

   where M_u represents the mass load of unit u. It is assumed in this work that the mass load of a water-using operation remains constant at the *given* nominal level. In addition, the upper limits of inlet and outlet concentrations must be imposed, i.e.,

   $$CI_u \le CI_u^U, \quad u \in \mathbb{U} \tag{17}$$

   $$CO_u \le CO_u^U, \quad u \in \mathbb{U} \tag{18}$$

   where CI_u^U and CO_u^U denote the corresponding maximum pollutant concentrations.
2. *Water treatment units*: The *removal ratio* is adopted in this work as the performance indicator of a water treatment operations. In particular, the component balance can be expressed as

   $$CI_t(1 - RR_t) = CO_t, \quad t \in \mathbb{T} \tag{19}$$

   where RR_t denotes the removal ratio of unit t and it is treated as a given constant. For every treatment unit, inequality constraints are usually imposed upon the throughput and the pollutant concentration at the inlet, i.e.,

   $$F_t \le F_t^U, \quad t \in \mathbb{T} \tag{20}$$

   $$CI_t \le CI_t^U, \quad t \in \mathbb{T} \tag{21}$$

   where F_t^U denotes the maximum allowable throughput of unit t, CI_t^U denotes the upper bound of pollutant concentration at the inlet of unit t.

2.3. Generalized formulation of flexibility index model

Decision making in the presence of uncertainty is a very important issue in process synthesis, since at this early stage decisions have to be made with limited knowledge of external disturbances. The traditional approach to deal with uncertainty is to first generate the system design based on the nominal values of process parameters and then introduce enough tolerance margins. These safety factors are usually determined on the basis of experience and/or intuition, and may lead to infeasible design solutions. Several approaches have already been developed to address this problem and the one proposed by Swaney and Grossmann (1985a, b) is adopted here. Specifically, these authors introduced the concept of *flexibility index*, which is a single scalar measure of the allowable variations in all uncertain parameters. A thorough treatment of this issue can be found in Biegler et al. (1997). For illustration clarity and completeness, the basic formulation of flexibility index model is still reviewed the sequel.

First, let us define the label sets for equality and inequality constraints respectively:

$$\mathbb{I} = \{i | i \text{ is the label of an equality constraint}\} \tag{22}$$

$$\mathbb{J} = \{j | j \text{ is the label of an inequality constraint}\} \tag{23}$$

The aforementioned general design model can then be expressed accordingly as

$$h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0, \quad i \in \mathbb{I} \tag{24}$$

$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \le 0, \quad j \in \mathbb{J} \tag{25}$$

where h_i is the i th equality constraint in the design model (e.g., the mass balance equation for a processing unit), g_j is the j th inequality constraint in the design model (e.g., a capacity limit), $\mathbf{d}$ represents a vector in which all design variables are stored, $\mathbf{z}$ denotes the vector of adjustable control variables, $\mathbf{x}$ is the vector of state variables, $\boldsymbol{\theta}$ denotes the vector of uncertain parameters.

Next, let us formulate a mathematical program to determine the feasibility function $\psi(\mathbf{d},\theta)$:

$$\psi(\mathbf{d},\theta)=\min_{\mathbf{z}}\max_{j\in\mathbb{J}} g_j(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) \tag{26}$$

s.t.

$$h_i(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta})=0, \quad i\in\mathbb{I} \tag{27}$$

Notice that the min–max term in Eq. (26) means that, for *fixed* design $\mathbf{d}$ and *fixed* parameters $\boldsymbol{\theta}$, the largest g_j $(\forall j\in\mathbb{J})$ is minimized by adjusting the control variables in $\mathbf{z}$. If $\psi(\mathbf{d},\theta)\le 0$, then the operation of given water network should be considered as feasible. Notice also that, if $\psi(\mathbf{d},\theta)=0$, then at least one of the inequality constraints is on the boundary of feasible region, i.e., $g_j=0$ $(\exists j\in\mathbb{J})$, and they are referred to as the *active constraints*.

Since every uncertain parameter in $\boldsymbol{\theta}$ may assume a value within the *given* interval, the corresponding parameter space Γ can be characterized as:

$$\Gamma=\{\boldsymbol{\theta}|\boldsymbol{\theta}^N-\Delta\boldsymbol{\theta}^-\le\boldsymbol{\theta}\le\boldsymbol{\theta}^N+\Delta\boldsymbol{\theta}^+\} \tag{28}$$

where $\boldsymbol{\theta}^N$ denotes the vector of nominal parameter values; $\Delta\boldsymbol{\theta}^+$ and $\Delta\boldsymbol{\theta}^-$ denote the vectors of expected deviations in the positive and negative directions respectively.

Since Eqs. (26) and (27) only work at fixed parameter values, we also need a feasibility criterion for *all* possible values in Γ. Hence, another optimization problem can be formulated to facilitate this decision:

$$\chi(\mathbf{d})=\max_{\boldsymbol{\theta}\in\Gamma}\psi(\mathbf{d},\boldsymbol{\theta}) \tag{29}$$

where $\chi(\mathbf{d})$ denotes the feasibility function of design $\mathbf{d}$ over the range Γ. The given system should therefore be feasible if $\chi(\mathbf{d})\le 0$, but infeasible if otherwise.

According to Swaney and Grossmann (1985a, b), the flexibility index can be regarded as a measure of the maximum tolerable range of variation in every uncertain parameter. Specifically, a feasible parameter space can be expressed as

$$\Gamma(\delta)=\{\boldsymbol{\theta}^N-\delta\Delta\boldsymbol{\theta}^-\le\boldsymbol{\theta}\le\boldsymbol{\theta}^N+\delta\Delta\boldsymbol{\theta}^+\} \tag{30}$$

where $\delta\ge 0$ is a scalar variable. Based on this definition, the flexibility index model can be formulated as follows:

$$F=\max\delta \tag{31}$$

s.t.

$$\chi(\mathbf{d})\le 0 \tag{32}$$

where F is referred to as the *flexibility index*, which is the largest value of δ that guarantees $g_j\le 0$ $(\forall j\in\mathbb{J})$, i.e., $\chi(\mathbf{d})\le 0$, in the parameter space $\Gamma(F)$.

The implementation procedure of above model is generally complicated because Eqs. (31) and (32) represent a nonlinear, non-differentiable, multilevel optimization problem. Grossmann and Floudas (1987) developed an alternative solution technique, which is called the *active set method*, according to the Karush–Kuhn–Tucker (KKT) conditions of the function $\psi(\mathbf{d},\theta)$. To be able to apply these conditions, the aforementioned flexibility index model is first reformulated to ensure $\psi(\mathbf{d},\theta)=0$:

$$F=\min\delta \tag{33}$$

s.t.

$$\psi(\mathbf{d},\theta)=0 \tag{34}$$

Notice that the original maximization problem is now replaced with a minimization problem. This is due to the fact that only the smallest value of δ is needed to cause one (or more) inequality constraint(s) g_j to be on the boundary exactly, i.e., $\psi(\mathbf{d},\theta)=0$. Since the function $\psi(\mathbf{d},\theta)$ must satisfy Eqs. (26) and (27), the corresponding KKT conditions should also be applicable. Consequently, the flexibility index problem in Eqs. (33) and (34) can be written more explicitly as the following nonconvex mixed-integer nonlinear program (MINLP):

$$F=\min_{\delta,\mu_i,\lambda_j,s_j,y_j,x_i,z_k}\delta \tag{35}$$

s.t.

$$h_i(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta})=0, \quad i\in\mathbb{I}$$

$$g_j(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta})+s_j=0, \quad j\in\mathbb{J}$$

$$\begin{aligned}&\sum_{j\in\mathbb{J}}\lambda_j=1\\&\sum_{i\in\mathbb{I}}\mu_i\frac{\partial h_i}{\partial\mathbf{z}}+\sum_{j\in\mathbb{J}}\lambda_j\frac{\partial g_j}{\partial\mathbf{z}}=0\\&\sum_{i\in\mathbb{I}}\mu_i\frac{\partial h_i}{\partial\mathbf{x}}+\sum_{j\in\mathbb{J}}\lambda_j\frac{\partial g_j}{\partial\mathbf{x}}=0\end{aligned} \tag{36}$$

$$\left.\begin{aligned}&s_j-Q(1-y_j)\le 0\\&\lambda_j-y_j\le 0\\&s_j\ge 0,\lambda_j\ge 0,y_j\in\{0,1\}\end{aligned}\right\}j\in\mathbb{J}$$

$$\theta^N-\delta\Delta\theta^-\le\theta\le\theta^N+\delta\Delta\theta^+,\quad \delta\ge 0$$

where s_j is the slack variable for the j th inequality constraint, i.e., s_j equals the difference between zero and g_j, Q denotes a large enough positive number to be used as the upper bound of s_j, μ_i denotes the Lagrange multiplier of equality constraint h_i, λ_j is the Lagrange multiplier of inequality constraint g_j, y_j denotes the binary variable reflecting whether the corresponding inequality constraint is active, i.e., $g_j=0$ if $y_j=1$, while $g_j<0$ if $y_j=0$.

2.4. Implementation procedure

To evaluate the flexibility index of an existing water network, it is necessary to introduce the following adjustments to the above generalized model:

1. *Incorporate uncertain multipliers into the general design model.* It is assumed in this work that a subset of the following parameters may be uncertain: the upper limit of primary water supply ($F_{w_1}^U$), the secondary water supply (F_{w_2}), the water source quality (C_w), the mass load of water-using unit (M_u) and the maximum inlet and outlet concentrations (CI_u^U and CO_u^U), the removal ratio of wastewater treatment unit (RR_t) and the upper bounds for inlet concentration (CI_t^U) and throughput (F_t). To characterize uncertainties in these parameters, additional multipliers are introduced into the design model, i.e.,

$$F_{w_1}^U=\overline{F}_{w_1}^U\theta_{F_{w_1}^U}, \quad w_1\in\mathbb{W}_1 \tag{37}$$

$$F_{w_2}=\overline{F}_{w_2}\theta_{F_{w_2}}, \quad w_2\in\mathbb{W}_2 \tag{38}$$

$$C_w=\overline{C}_w\theta_{C_w}, \quad w\in\mathbb{W} \tag{39}$$

$$M_u=\overline{M}_u\theta_{M_u}, \quad u\in\mathbb{U} \tag{40}$$

$$CI_u^U=\overline{CI}_u^U\theta_{CI_u^U}, \quad u\in\mathbb{U} \tag{41}$$

$$CO_u^U = \overline{CO}_u^U \theta_{CO_u^U}, \quad u \in \mathbb{U} \tag{42}$$

$$RR_t = \overline{RR}_t \theta_{RR_t}, \quad t \in \mathbb{T} \tag{43}$$

$$CI_t^U = \overline{CI}_t^U \theta_{CI_t^U}, \quad t \in \mathbb{T} \tag{44}$$

$$F_t = \overline{F}_t^U \theta_{F_t^U}, \quad t \in \mathbb{T} \tag{45}$$

where, $\overline{F}_{w_1}^U$, $\overline{F}_{w_2}$, $\overline{C}_w$, $\overline{M}_u$, $\overline{CI}_u^U$, $\overline{CO}_u^U$, $\overline{RR}_t$, $\overline{CI}_t^U$ and $\overline{F}_t^U$ denote the nominal values of the above-mentioned uncertain parameters, and $\theta_{F_{w_1}^U}$, $\theta_{F_{w_2}}$, θ_{C_w}, θ_{M_u}, $\theta_{CI_u^U}$, $\theta_{CO_u^U}$, θ_{RR_t}, $\theta_{CI_t^U}$ and $\theta_{F_t^U}$ are the corresponding uncertain multipliers. Notice that the nominal parameter values should be considered as given constants in the flexibility index model. The uncertain multipliers are assumed to be located within the parameter space defined by Eq. (30), in which all nominal multiplier values equal one and the positive and negative deviations, i.e., $\Delta\boldsymbol{\theta}^+$ and $\Delta\boldsymbol{\theta}^-$, are given. Notice also that Eqs. (37)–(45) can be substituted into the general design model, i.e., Eqs. (8)–(21), and then used as the equality and inequality constraints of the flexibility index model, i.e., Eqs. (24) and (25), for water networks.

2. *Impose additional equality constraints to stipulate the no-flow conditions in missing branches.* In a given water network design, not all branches in the superstructure are present. The flow rates in the nonexistent branches should therefore be set to zero. These new equations must then be augmented with those in the general design model and treated as the equality constraints in the flexibility index model given in Eq. (24).
3. *Construct the flexibility index model for the given water network.* This step can be carried out by directly substituting the equality and inequality constraints obtained in the previous two steps into Eq. (36).

2.5. Additional performance evaluation criterion

Since only two types of structural modifications are considered in this study, alternative revamp designs may not be clearly differentiated from one another according to their flexibility levels and/or the required capital expenditures. The minimum operating cost of each design is also computed in this study for use as an additional performance evaluation criterion. Specifically, the objective function of the corresponding optimization problem can be expressed as

$$\min\left(F_{w_1}\gamma_{w_1} + \sum_{t \in \mathbb{T}} F_t\gamma_t + \sum_{s \in \mathbb{S}} F_s\gamma_s\right), \quad w_1 \in \mathbb{W}_1 \tag{46}$$

where γ_{w_1} is the unit cost of freshwater obtained from sources w_1, γ_t is the unit cost for water treatment in unit t, and γ_s is the unit cost for discharging wastewater to sink s.

3. Solution strategies of flexibility index model

The flexibility index model formulated in the previous section is very difficult to solve in practice. Effective solution strategies are therefore needed to improve convergence rate and to produce sufficiently satisfactory optima. To this end, an elaborated procedure has been developed in this work for use in the GAMS environment. A detailed description is provided below.

3.1. Smoothing function

By utilizing the hyperbolic approximation technique proposed by Biegler and Balakrishna (1992), the smoothing function method (Bandoni et al., 2000) can be applied to convert the original MINLP model, i.e., Eqs. (35) and (36), into an alternative nonconvex nonlinear program (NLP):

$$F = \min_{\delta,\mu_i,\lambda_j,x_i,z_k} \delta \tag{47}$$

s.t.

$$h_i(\mathbf{d},\mathbf{z},\mathbf{x},\boldsymbol{\theta}) = 0, \quad i \in \mathbb{I}$$

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

$$\sum_{j \in \mathbb{J}} \lambda_j = 1$$

$$\sum_{i \in \mathbb{I}} \mu_i \frac{\partial h_j}{\partial \mathbf{z}} + \sum_{j \in \mathbb{J}} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} = 0$$

$$\sum_{i \in \mathbb{I}} \mu_i \frac{\partial h_j}{\partial \mathbf{x}} + \sum_{j \in \mathbb{J}} \lambda_j \frac{\partial g_j}{\partial \mathbf{x}} = 0$$

$$\lambda_j - \tfrac{1}{2}[(\sqrt{(\lambda_j+g_j)^2+\varepsilon^2}) + \lambda_j + g_j] = 0, \quad \lambda_j \ge 0$$

$$\theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+, \quad \delta \ge 0 \tag{48}$$

Because the smoothing method is basically an approximation technique, this approach inevitably produces local solutions which may not be identical to those obtained with the original MINLP formulation. The validity of this approximation strategy depends largely on the magnitude of the chosen parameter ε. A smaller ε yields more accurate solution, but may cause ill-conditioning. Since in general the solution process of a NLP model converges faster, the corresponding results can be used as a good initial guess for solving the MINLP model.

3.2. Initialization method

The task of initialization is of critical importance for solving optimization problems because the workload involved in finding an appropriate optimal solution may be reduced by identifying infeasible ones that satisfy (or closely satisfy) most constraints. If the initial guess is close to the global optimum, the iteration process may be shortened considerably. In addition, notice that the non-convex models may have multiple solutions. If the search procedure starts in the right neighborhood, it is more likely to end up with a desired solution. The following initialization procedure has been found to be effective in our case studies.

Step 1: *produce the initial values of the process variables by solving a nonlinear program that minimizes freshwater usage.*

A nonlinear programming model can be constructed to minimize the freshwater usage in the given water network, i.e.,

$$\min F_{w_1}, \quad w_1 \in \mathbb{W}_1 \tag{49}$$

subject to the equality and inequality constraints specified in the general design model, i.e., Eqs. (8)–(21), and also the zero-flow constraints for the nonexistent branches. Notice that all uncertain parameters should be fixed at their nominal levels in this model. Although other objective functions can obviously be used also, it has been found in our study that this approach yields somewhat better convergence behavior and more convenient initial settings for variables not included in this NLP model.

Since the constraints used in the above NLP model are also included in the flexibility index model, the optimum solution of the former model must be a feasible one of the latter. It should be further noted that, if we set the upper bound of freshwater supply rate in the flexibility index model to be at the minimum level, then no uncertain disturbances can be allowed and $\delta = 0$. In other words, the optimum solution of the aforementioned NLP should be regarded as a feasible solution of the flexibility index model with *no flexibility*.

Because the proposed NLP model is in general easier to solve, the optimization computations often converge successfully with initial values generated by a brute-force strategy. Specifically, multiple initial values can be generated arbitrarily with a random number generator for each decision variable. The optimization results of the corresponding runs can then be compared to ensure that a near global optimum is reached. It should also be noted that not all initial values can be obtained in the present step. In particular, only the optimum values of the following variables can be identified: F_{w_1} ($w_1 \in \mathbb{W}_1$), F_p ($p \in \mathbb{P}$), CI_p ($p \in \mathbb{P}$), CO_p ($p \in \mathbb{P}$), F_s ($s \in \mathbb{S}$), $f_{w,p}$ ($w \in \mathbb{W}$, p $\in \mathbb{P}$), $f_{p,p'}$ ($p, p' \in \mathbb{P}$), $f_{w_2,s}$ ($w_2 \in \mathbb{W}_2, s \in \mathbb{S}$), and $f_{p,s}$ ($p \in \mathbb{P}, s \in \mathbb{S}$).

Step 2: *set the initial values of flexibility index and uncertain multipliers*.

Based on the discussions given in the previous step, these initial values should be

$$\delta^{iv} = 0 \tag{50}$$

$$\theta^{iv}_{M_u} = \theta^{iv}_{C_w} = \theta^{iv}_{RR_t} = \theta^{iv}_{CI^U_u} = \theta^{iv}_{CI^U_t} = \theta^{iv}_{CO^U_u} = \theta^{iv}_{F^U_t} = \theta^{iv}_{C^U_s} = 1 \tag{51}$$

where $u \in \mathbb{U}$, $w \in \mathbb{W}$, $t \in \mathbb{T}$, $u \in \mathbb{U}$, $t \in \mathbb{T}$, $u \in \mathbb{U}$, $t \in \mathbb{T}$ and $s \in \mathbb{S}$.

Step 3: *generate the initial values of lagrange multipliers with random number generators*.

The initial values of Lagrange multipliers for the inequality constraints, i.e., λ_j, can be generated according to the following method:

$$\lambda^{iv}_j = \begin{cases} 0 & \text{if } g^{iv}_j > 0 \\ \text{rand}(0,1) & \text{if } g^{iv}_j < 0 \end{cases}, \quad j \in \mathbb{J} \tag{52}$$

where rand(α, β) denotes an operator yielding a random number between α and β. On the other hand, the initial values of Lagrange multipliers for equality constraints, i.e., μ_i, were created with the following approach:

$$\mu^{iv}_i = \text{rand}(-Z, Z), \quad i \in \mathbb{I} \tag{53}$$

where Z is a sufficiently large positive number, which can be set between 1000 and 10 000 in most cases.

It should be pointed out that the above three steps should be enough for initializing the flexibility index model with smoothing functions. For the original MINLP formulation, a fourth step is needed.

Step 4: *determine the initial values of slack variables and binary variables.*

These values can be calculated with the following formulas:

$$s^{iv}_j = -g^{iv}_j \tag{54}$$

$$y^{iv}_j = \begin{cases} 0 & \text{if } \lambda^{iv}_j = 0 \\ 1 & \text{if } \lambda^{iv}_j > 0 \end{cases} \tag{55}$$

where $j \in \mathbb{J}$. Notice that this step can be applied as the continuation of the first three steps, or as a follow-up procedure after a preliminary solution of the flexibility index model is obtained with the smoothing functions. As noted previously, this preliminary solution is also a good starting point for solving the original formulation.

3.3. Search algorithm

A comprehensive search algorithm has been developed in this work to identify the optimal solution of flexibility index model. The proposed solution procedure can be implemented in two stages. The first stage is designed to generate a set of initial values by minimizing the freshwater usage in the given water network. To properly determine the flexibility index with these initial values, one or both of the two alternative formulations described previously, i.e., the nonconvex NLP and MINLP models obtained with and without the smoothing approximation, may be utilized in the second stage. It should also be emphasized that the solution steps in both stages can be incorporated in a single GAMS code. The NLP problems are solved with CONOPT, while MINLP with BARON. The flowchart of this algorithm can be found in Fig. 1. Brief explanations are provided in the sequel:

Stage 1: For illustration convenience, the mathematical programming model used in this stage will be referred to as the *freshwater usage minimization* (FUM) model. Every new feasible solution found in the iteration process is compared with the best one obtained in the previous iterations. If the new objective value is lower, then the latter should be replaced with former. Note that it is very important to set large enough iteration limit to ensure that a near global minimum is reached. The local minimums may lead to erroneous search results in the second stage.

Stage 2: As mentioned previously, the flexibility index can be computed with either a mixed-integer nonlinear programming model or a nonlinear programming model. For illustration convenience, the former is referred to as a MINLP FI model and the latter a NLP FI model.

Notice first that not all initial values required in the MINLP FI model can be generated in the first stage. Additional initial values for flexibility index, uncertainty multipliers, Lagrange multipliers, slack variables, and binary variables have to be produced first with the proposed methods. Notice also that the upper bound of flexibility index is renewed every time a new feasible solution can be identified. It has been observed that the convergence rate can be improved by setting this upper bound at a level slightly lower than that found in the prior iteration. A sufficiently large number (say 3–10) is used as the first upper bound in the iteration process.

If the attempt to solve the MINLP FI model is failed, the initial values obtained from the first stage are used again for solving the NLP FI model. If a feasible solution can be identified, the corresponding optimization output should be adopted as the improved initial guess for the MINLP FI model. Of course it is still necessary to produce the initial values of slack and binary variables to facilitate faster convergence.

If the feasible solution of NLP FI model fails to give satisfactory initial values for the MINLP FI model, this solution should be used instead as the input to a new NLP FI model, which can be formulated with a lower value of approximation parameter (ε). Since the new solution is believed to be more accurate than that obtained in the previous iteration, it should be considered as a better starting point for solving the MINLP FI model.

In general, it may be necessary to repeat the above iteration steps several times in order to reach the true optimum of the MINLP FI model. In setting the initial value of ε, the trade-off between computation efficiency and approximation accuracy must be considered. We found a value between 0.2 and 2 usually serve our propose well.

4. Revamp heuristics for enhancing flexibility

As mentioned previously, two classes of structural modifications are considered in this work, i.e., (1) inserting/deleting pipeline connections and (2) adding/replacing treatment units. In principle, it is possible to write a computer program to automatically search for the needed design modification with an auxiliary superstructure. However, this approach may not be justifiable since the required computation load can grow exponentially even for a small network and, also, we usually do not look for nor need a network design in revamp study which involves a drastic structural change. It is thus our intention to

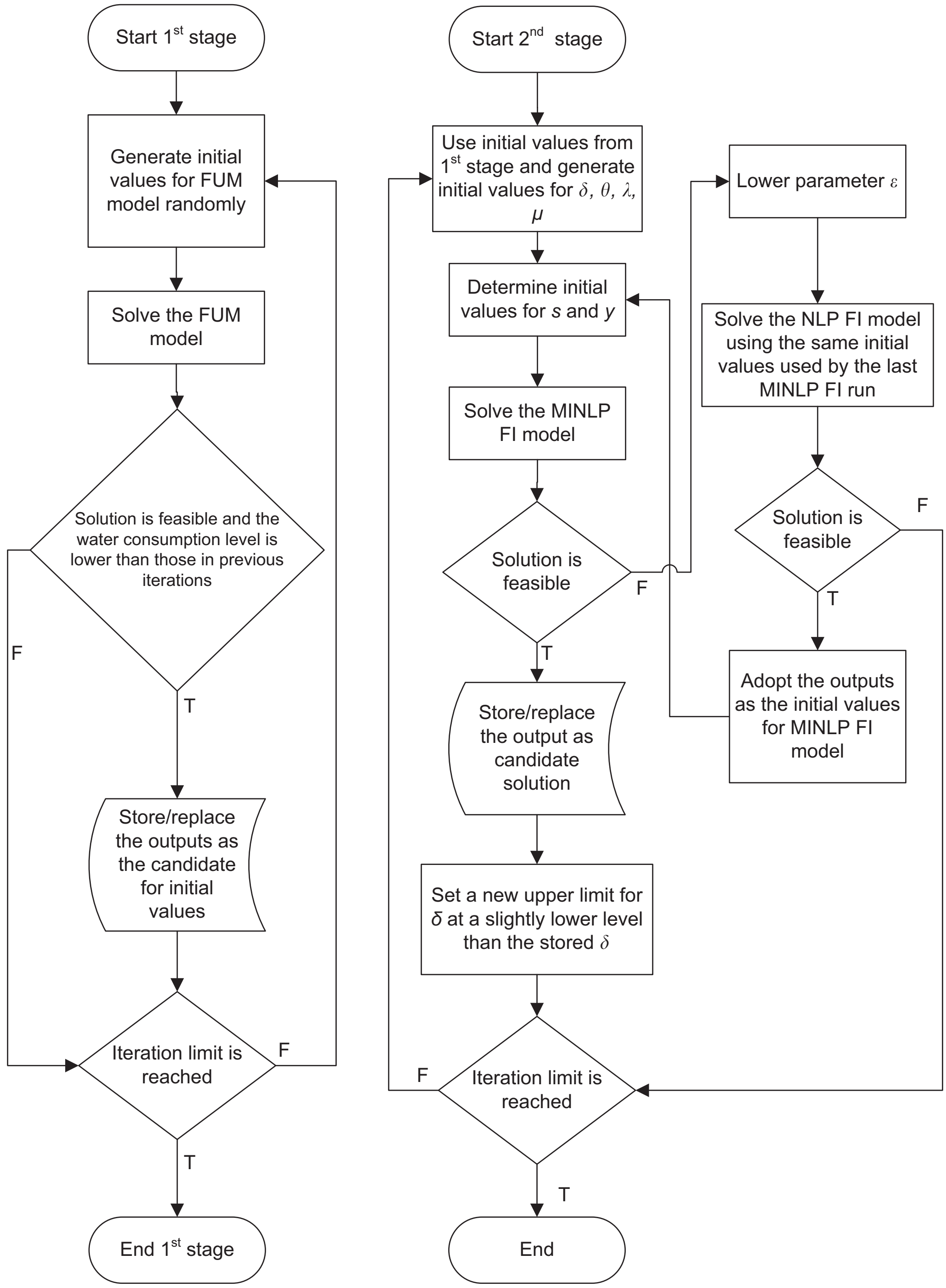

Fig. 1. Overall search algorithm.

heuristically identify an acceptable solution while keeping the size of optimization problem reasonably small. For this purpose, several effective heuristics have been developed in this study on the basis of a large volume of test-case results (Riyanto, 2009). These heuristic design rules are briefly summarized here and, in general, they should be implemented in the same order given below.

1. Introduce additional pipeline connection(s) to the nominal network so as to relax the active constraints in the solution of the original flexibility index model.
   (a) Send clean water to a water-using unit in order to relax its inlet concentration constraint. This water can be taken from a water treatment unit or a water-using unit.
   (b) Increase the throughput of a water-using unit in order to relax its outlet concentration constraint. A higher throughput may be achieved with clean enough water from another unit.
   (c) Send clean water to a water treatment unit in order to relax its inlet concentration constraint. As the output of treatment unit should be cleaner than it input, self recycle is a viable option.
   (d) Divert a portion of the water flow going into a sink to water treatment unit(s) so as to relax the concentration constraint at the sink. This action must be considered along with other constraints in the water network, such as the concentration and/or throughput constraints of the

treatment unit(s) at the receiving end, and also the constraints of the unit(s) further downstream.

2. Improve the performance of one or more existing treatment unit(s). This task can be accomplished by replacing old units with better ones, by implementing a more up-to-date technology, by adding a post-treatment unit, or simply by repairing the existing treatment unit which is not working so well. It should also be noted that this approach does not guarantee flexibility enhancement.
3. Place one or more new treatment unit to relax the active constraints described below:
   (a) Place them before a water-using unit to relax its inlet and/or outlet concentration constraints.
   (b) Place them in parallel with an existing unit to relieve its treatment load and to relax its active throughput constraint as well.
   (c) Place them on the effluent flows to relax the concentration constraint at the sink.

Notice that the above revamp options have been organized in a systematic revamp procedure and the corresponding flowchart can be found in Riyanto (2009). In addition, these options can be roughly divided into three general categories based on capital investment costs, i.e., (1) adding auxiliary pipelines, (2) upgrading existing treatment units, and (3) adding extra treatment units. Since their cost ranges are significantly different, these three types of design modifications can be attempted sequentially one-at-a-time according to the order stated above. On the other hand, if the same type of structural changes are being considered, they are ranked in this work on the basis of the corresponding minimum operating costs, i.e., Eq. (46).

5. Case studies

The results of several case studies are presented here to demonstrate the feasibility and benefits of the proposed revamp procedure.

5.1. Case I

Let us consider the nominal water network presented in Fig. 2, which is taken from Li et al. (2009) (Design 1 in Example 2). The corresponding model parameters and cost coefficients are presented in Table 1. The solution of flexibility index model for this network are presented in Table 2. Let us assume that the upper limit of freshwater supply rate cannot exceed 30 t/h. Under this condition, Table 2 presents that the nominal network may not be resilient enough since the corresponding flexibility index is only 0.32. Due to budget constraint, it is also assumed in this example that new treatment units cannot be added to improve the system performance. From the values of the binary variables y_j, it is clear that the active constraints are associated with $\overline{F}_{w1}^U$, $\overline{F}_{t1}^U$, $\overline{F}_{t2}^U$, $\overline{CI}_{u1}^U$, $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, and $\overline{C}_{s1}^U$. In addition, it should be noted that only the last four of these active constraints may be relaxed with auxiliary pipelines. Let us first analyze those possibilities:

1. Constraint $\overline{CI}_{u1}^U$: The inlet concentration of unit $u1$ cannot be lowered by adding new connections from other processing units, as the only flow with an acceptable concentration level, i.e., less than $\overline{CI}_{u1}^U$ (1 ppm), is the freshwater (0.1 ppm).
2. Constraint $\overline{CO}_{u1}^U$: This constraint may be relaxed if $u1$ is operated at a higher throughput level. However, such a requirement cannot be satisfied with auxiliary pipelines since the constraint associated with $\overline{CI}_{u1}^U$ is already active and, on the basis of the argument against the revamp action mentioned above, it is not possible to find any secondary water source with concentration lower than 1 ppm. Therefore, the present revamp option should be abandoned.
3. Constraint $\overline{CO}_{u2}^U$: It may be possible to relax this constraint since the inlet concentration of $u2$ in the nominal design does not reach its upper bound. A new connection is thus added from $u1$

Table 1
The model parameters in case I.

Parameters		Values	Parameters		Values
$\overline{F}_{w1}^U$	(t/h)	30.000	$\Delta\theta_{C_{w2}}^+$		0.100
$\overline{F}_{w2}$	(t/h)	30	$\Delta\theta_{C_{w2}}^-$		0.100
$\overline{C}_{w1}$	(ppm)	0.100	$\Delta\theta_{M_{u1}}^+$		0.150
$\overline{C}_{w2}$	(ppm)	150.000	$\Delta\theta_{M_{u1}}^-$		0.150
$\overline{CI}_{u1}^U$	(ppm)	1.000	$\Delta\theta_{M_{u2}}^+$		0.150
$\overline{CI}_{u2}^U$	(ppm)	80.000	$\Delta\theta_{M_{u2}}^-$		0.150
$\overline{CI}_{u3}^U$	(ppm)	50.000	$\Delta\theta_{M_{u3}}^+$		0.150
$\overline{CI}_{t1}^U$	(ppm)	185.000	$\Delta\theta_{M_{u3}}^-$		0.150
$\overline{CI}_{t2}^U$	(ppm)	200.000	$\Delta\theta_{RR_{t1}}^+$		0.030
$\overline{CO}_{u1}^U$	(ppm)	101.000	$\Delta\theta_{RR_{t1}}^-$		0.030
$\overline{CO}_{u2}^U$	(ppm)	240.000	$\Delta\theta_{RR_{t2}}^+$		0.030
$\overline{CO}_{u3}^U$	(ppm)	200.000	$\Delta\theta_{RR_{t2}}^-$		0.030
$\overline{C}_{s1}$	(ppm)	10.000			
$\overline{F}_{t1}^U$	(t/h)	125.000			
$\overline{F}_{t2}^U$	(t/h)	135.000			
$\overline{M}_{u1}$	(kg/h)	4.000	Cost coefficients		
$\overline{M}_{u2}$	(kg/h)	5.600	γ_{w1}	(\$/t)	1
$\overline{M}_{u3}$	(kg/h)	4.500	γ_{t1}	(\$/t)	2
$\overline{RR}_{t1}$		0.9	γ_{t2}	(\$/t)	1
$\overline{RR}_{t2}$		0.8	γ_{s1}	(\$/t)	0

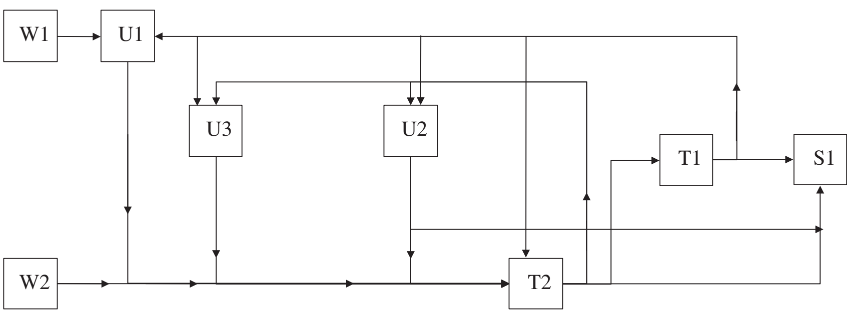

Fig. 2. Nominal structure of water network in case I.

to $u2$ as the water flow from $u1$ is the cleanest among all three water-using units and, also, all treatment units have already been connected to $u2$. For convenience, this revamp option is referred to as design I-A in this paper. It was determined that the flexibility index of design I-A is the same as that of the original structure. This is due to the fact that the outlet stream of unit $u1$ is much dirtier than the inlet of unit $u2$.

4. Constraint $\overline{C}_{s1}^U$: None of the flows heading towards sink $s1$ can be diverted to the treatment units as they are all at their throughput limits.

The second stage of the revamp procedure is to improve the separation efficiencies of existing treatment units. Let us consider two scenarios where the removal ratios of $t1$ and $t2$ can be raised to 0.95 (design I-B) and 0.85 (design I-C) respectively. Notice that the structures of both designs are the same as the nominal network and the corresponding flexibility indices can be increased respectively to 0.964 for design I-B and 0.650 for design I-C. This is because in these networks cleaner waters can be produced with better treatment units and, consequently, cleaner inputs can be used in all water-using units and sink. As a result, the constraints associated with $\overline{CI}_{u1}^U$, $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, and $\overline{C}_{s1}^U$ can be relaxed simultaneously.

Next let us consider the possibility of augmenting design I-B or design I-C with additional auxiliary pipelines. According to the above discussions, one can see that it is only possible to relax the active constraint associated with $\overline{CO}_{u2}^U$ in the original model by adding auxiliary pipelines. Since the network structures of design I-B and I-C are identical to that of the nominal design and there are no new active constraints, it can be expected that the only relaxable constraint is again associated with $\overline{CO}_{u2}^U$. Since this constraint is not active in design I-B, it is only necessary to evaluate the benefit of adding a connection from $u1$ to $u2$ in design I-C (which will be referred to as design I-D). It can be observed that the flexibility levels of design I-C and I-D are the same. The argument applied to explain why design I-A fails to achieve a better performance over the nominal design, i.e., the positive effect of increasing throughput of unit $u2$ is canceled out by the increase in inlet concentration, is also applicable in the present case.

Our last resort (design I-E) is a combination of design I-B and design I-C. The optimization results show that the corresponding flexibility index can be improved to 1.478. This indicates that design I-E should be a suitable revamp candidate for the present case study.

Table 2
The solution of flexibility index model obtained with nominal network design in case I.

Results		Values	Results		Values
$f_{w1,u1}$	(t/h)	30.000	$y_{F_{w1}^U}$		1
$f_{w2,t2}$	(t/h)	30.000	$y_{CI_{u1}^U}$		1
$f_{u1,t2}$	(t/h)	41.921	$y_{CI_{u2}^U}$		0
$f_{u2,t2}$	(t/h)	24.116	$y_{CI_{u3}^U}$		0
$f_{u2,s1}$	(t/h)	0.676	$y_{CI_{t1}^U}$		0
$f_{u3,t2}$	(t/h)	38.963	$y_{CI_{t2}^U}$		0
$f_{t1,u1}$	(t/h)	11.921	$y_{CO_{u1}^U}$		1
$f_{t1,u2}$	(t/h)	24.791	$y_{CO_{u2}^U}$		1
$f_{t1,u3}$	(t/h)	38.079	$y_{CO_{u3}^U}$		0
$f_{t1,s1}$	(t/h)	50.208	$y_{C_{s1}^U}$		1
$f_{t2,u3}$	(t/h)	0.883	$y_{F_{t1}^U}$		1
$f_{t2,t1}$	(t/h)	125.000	$y_{F_{t2}^U}$		1
$f_{t2,s1}$	(t/h)	9.117			
CI_{u1}	(ppm)	1.000			
CI_{u2}	(ppm)	3.265			
CI_{u3}	(ppm)	3.872			
CI_{t1}	(ppm)	30.050			
CI_{t2}	(ppm)	144.689			
CO_{u1}	(ppm)	101.000			
CO_{u2}	(ppm)	240.000			
CO_{u3}	(ppm)	124.916			
CO_{t1}	(ppm)	3.265			
CO_{t2}	(ppm)	30.050	Minimized operation cost	(\$/h)	266.137
C_{s1}	(ppm)	10.000	Flexibility index		0.320

5.2. Case II

Let us consider the water network presented in Fig. 3, which is also taken from Li et al. (2009) (design 3 in example 2). The model parameters and the cost coefficients adopted in the present example are the same as those used in case I (see Table 1). Let us assume that the upper limit of freshwater supply rate also cannot exceed 30 t/h. The optimal solution of the corresponding flexibility index model is presented in Table 3. Notice that this nominal network is not flexible enough since δ reaches only 0.387. The active constraints in this case are those associated with $\overline{F}_{w1}^U$, $\overline{F}_{t1}^U$, $\overline{F}_{t2}^U$, $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, $\overline{CO}_{u3}^U$ and $\overline{C}_{s1}^U$, while only the last four may be relaxed by adding auxiliary pipelines. Let us evaluate these possibilities first:

1. Constraints $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, and $\overline{CO}_{u3}^U$: The active outlet concentration constraint of a water-using unit can be relaxed by introducing an additional clean water flow to increase its throughput. The water flows from treatment units in this example cannot be selected for this purpose as all of them are used to maintain the active constraints on other units and/or sink. Specifically, the output from $t1$ is needed to maintain the constraints for $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, $\overline{CO}_{u3}^U$ and $\overline{C}_{s1}$, while the output from $t2$ is needed for $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, and $\overline{C}_{s1}$. Sharing these flows will inevitably result in a lower flexibility level. Thus, the output

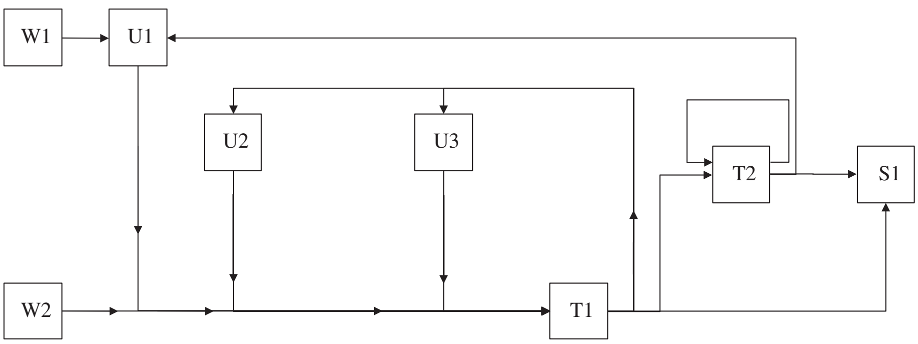

Fig. 3. Nominal structure of water network in case II.

from unit $u1$ is chosen to be the water source for increasing the throughputs of $u2$ and $u3$ since its concentration is the lowest among all eligible candidates. In addition, unit $u1$ is a bad choice to be considered as the recipient of additional flow since its inlet concentration limit is very low (1 ppm).

A revamp design is generated by adding a pipeline from unit $u1$ to unit $u2$ (design II-A), and another by adding the connection from $u1$ to $u3$ (design II-B). The optimal solutions of the corresponding flexibility index models show that these design options raise the flexibility index to 1.150 for design II-A, and 0.658 for design II-B. In the former case, although the revamp action significantly causes an increase in the inlet concentration of unit $u2$, the active constraint corresponding to $\overline{CO}^U_{u2}$ is relaxed due to the increase of throughput in unit $u2$ (42.340 t/h in design II-A versus 26.713 t/h in the nominal design). On the other hand, the flexibility level of design II-B is also improved significantly, although not enough to reach the desired level of 1. It appears that, although constraint for $\overline{CO}^U_{u3}$ is relaxed, the constraint associated with $\overline{CO}^U_{u2}$ is still active.

To confirm that the exit flow from unit $u1$ is indeed the best candidate for use as the needed additional water source, we have also tried to determine the effects of connecting unit $u3$ to $u2$ (design II-C). The solution of the corresponding model shows that the flexibility index of design II-C (0.535) is smaller than those achieved in designs II-A and II-B. The optimal solution from the corresponding flexibility index model also shows that the active constraints in all three cases are the same except an extra one, i.e., that associated with $\overline{CI}^U_{u2}$, is embedded in design II-C. This finding reveals that, although adding a connection from $u3$ to $u2$ is capable of relaxing the constraint for $\overline{CO}^U_{u2}$, the constraint for $\overline{CI}^U_{u2}$ becomes a new bottleneck which prevents design II-C from further improving its flexibility level. This is not a problem in design II-A since the pollutant concentration of the water flow from unit $u1$ is much lower than that from $u3$.

2. Constraint $\overline{C}^U_{s1}$: The water flows heading towards sink $s1$ cannot be diverted to the treatment units as they are at their throughput limits.

Since in this case it has already been shown that design II-A is capable of compensating the anticipated disturbances, it is not necessary to further consider upgrading/replacing treatment units. Our final selection in this example, i.e., design II-A, is presented in Fig. 4.

Table 3
The solution of flexibility index model obtained with nominal network design in case study II.

Results		Values	Results		Values
$f_{w1,u1}$	(t/h)	30.000	$y_{F^U_{w1}}$		1
$f_{w2,t1}$	(t/h)	30.000	$y_{CI^U_{u1}}$		0
$f_{u1,t1}$	(t/h)	42.098	$y_{CI^U_{u2}}$		0
$f_{u2,t1}$	(t/h)	26.713	$y_{CI^U_{u3}}$		0
$f_{u3,t1}$	(t/h)	26.188	$y_{CI^U_{t1}}$		0
$f_{t1,u2}$	(t/h)	26.713	$y_{CI^U_{t2}}$		0
$f_{t1,u3}$	(t/h)	26.188	$y_{CO^U_{u1}}$		1
$f_{t1,t2}$	(t/h)	41.284	$y_{CO^U_{u2}}$		1
$f_{t1,s1}$	(t/h)	30.814	$y_{CO^U_{u3}}$		1
$f_{t2,u1}$	(t/h)	12.098	$y_{C^U_{s1}}$		1
$f_{t2,t2}$	(t/h)	93.716	$y_{F^U_{t1}}$		1
$f_{t2,s1}$	(t/h)	29.186	$y_{F^U_{t2}}$		1
CI_{u1}	(ppm)	0.463			
CI_{u2}	(ppm)	18.182			
CI_{u3}	(ppm)	18.182			
CI_{t1}	(ppm)	164.601			
CI_{t2}	(ppm)	6.505			
CO_{u1}	(ppm)	101.000			
CO_{u2}	(ppm)	240.000			
CO_{u3}	(ppm)	200.000			
CO_{t1}	(ppm)	18.182			
CO_{t2}	(ppm)	1.362	Minimized operation cost	(\$/h)	307.265
C_{s1}	(ppm)	10.000	Flexibility index		0.387

5.3. Case III

Let us consider the nominal water network presented in Fig. 5, which consists of one freshwater source, one secondary water source, four water-using units, one treatment unit, and one sink. Other than the uncertain parameters discussed in the previous two cases, the random disturbances in freshwater supply rate ($\theta_{F^U_{w1}}$) and freshwater quality ($\theta_{C^U_{w1}}$) are also considered here. Let us

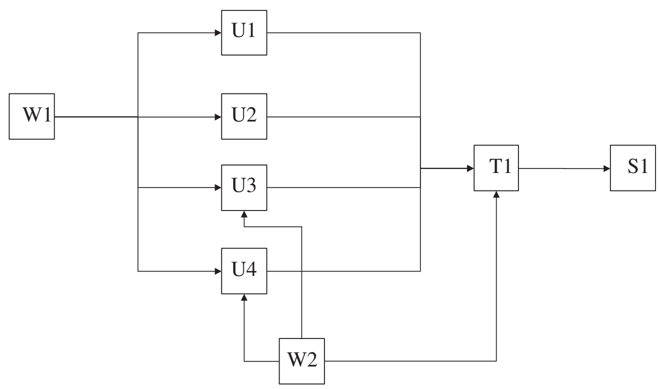

Fig. 5. Nominal structure of water network in case III.

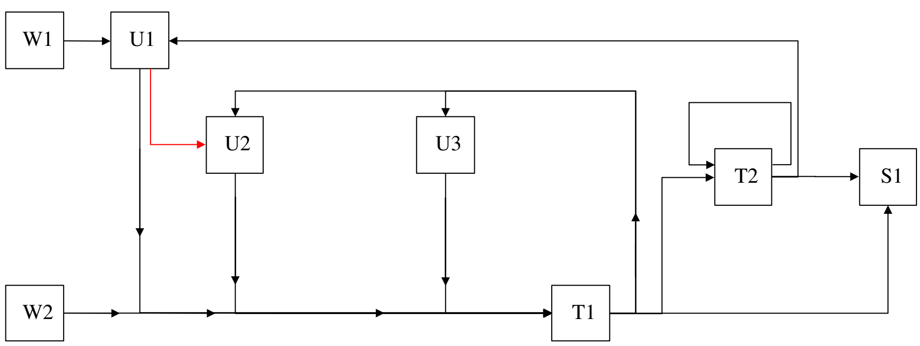

Fig. 4. Revamp design II-A.

Table 4
The model parameters in case III.

Parameters		Values	Parameters		Values
$\overline{F}_{w1}^U$	(t/h)	25	$\Delta\theta^+_{F^U_{w1}}$		0.100
$\overline{F}_{w2}$	(t/h)	100	$\Delta\theta^-_{F^U_{w1}}$		0.100
$\overline{C}_{w1}$	(ppm)	0.050	$\Delta\theta^+_{C_{w1}}$		0.100
$\overline{C}_{w2}$	(ppm)	100.000	$\Delta\theta^-_{C_{w1}}$		0.100
$\overline{CI}_{u1}^U$	(ppm)	1.000	$\Delta\theta^+_{C_{w2}}$		0.100
$\overline{CI}_{u2}^U$	(ppm)	50.000	$\Delta\theta^-_{C_{w2}}$		0.050
$\overline{CI}_{u3}^U$	(ppm)	100.000	$\Delta\theta^+_{M_{u1}}$		0.150
$\overline{CI}_{u4}^U$	(ppm)	100.000	$\Delta\theta^-_{M_{u1}}$		0.150
$\overline{CI}_{t1}^U$	(ppm)	200.000	$\Delta\theta^+_{M_{u2}}$		0.150
$\overline{CO}_{u1}^U$	(ppm)	50.000	$\Delta\theta^-_{M_{u2}}$		0.150
$\overline{CO}_{u2}^U$	(ppm)	250.000	$\Delta\theta^+_{M_{u3}}$		0.150
$\overline{CO}_{u3}^U$	(ppm)	200.000	$\Delta\theta^-_{M_{u3}}$		0.150
$\overline{CO}_{u4}^U$	(ppm)	200.000	$\Delta\theta^+_{M_{u4}}$		0.150
$\overline{C}_{s1}$	(ppm)	50.000	$\Delta\theta^-_{M_{u4}}$		0.150
$\overline{F}_{t1}^U$	(t/h)	125.000			
$\overline{M}_{u1}$	(kg/h)	0.100			
$\overline{M}_{u2}$	(kg/h)	2.000	Cost coefficients		
$\overline{M}_{u3}$	(kg/h)	5.000	γ_{w1}	(\$/t)	2
$\overline{M}_{u4}$	(kg/h)	7.000	γ_{t1}	(\$/t)	1
$\overline{RR}_{t1}$		0.8	γ_{s1}	(\$/t)	1.5

Table 5
The solution of flexibility index model obtained with nominal network design in case III.

Results		Values	Results		Values
$f_{w1,u1}$	(t/h)	2.077	$y_{F^U_{w1}}$		1
$f_{w1,u2}$	(t/h)	8.300	$y_{CI^U_{u1}}$		0
$f_{w1,u3}$	(t/h)	12.239	$y_{CI^U_{u2}}$		0
$f_{w1,u4}$	(t/h)	1.762	$y_{CI^U_{u3}}$		0
$f_{w2,u3}$	(t/h)	28.090	$y_{CI^U_{u4}}$		1
$f_{w2,u4}$	(t/h)	70.848	$y_{CI^U_{t1}}$		1
$f_{w2,t1}$	(t/h)	1.061	$y_{CO^U_{u1}}$		1
$f_{u1,t1}$	(t/h)	2.077	$y_{CO^U_{u2}}$		1
$f_{u2,t1}$	(t/h)	8.300	$y_{CO^U_{u3}}$		1
$f_{u3,t1}$	(t/h)	40.330	$y_{CO^U_{u4}}$		1
$f_{u4,t1}$	(t/h)	72.610	$y_{C^U_{s1}}$		0
$f_{t1,s1}$	(t/h)	124.378	$y_{F^U_{t1}}$		0
CI_{u1}	(ppm)	0.051			
CI_{u2}	(ppm)	0.051			
CI_{u3}	(ppm)	71.399			
CI_{u4}	(ppm)	100.000			
CI_{t1}	(ppm)	200.000			
CO_{u1}	(ppm)	50.000			
CO_{u2}	(ppm)	250.000			
CO_{u3}	(ppm)	200.000			
CO_{u4}	(ppm)	200.000			
CO_{t1}	(ppm)	40.000	Minimized operation cost	(\$/h)	342.273
C_{s1}	(ppm)	40.000	Flexibility index		0.249

assume that the upper limit of freshwater supply rate cannot exceed 25 t/h. The corresponding model parameters and cost coefficients are presented in Table 4, and the solution of flexibility index model for this network are presented in Table 5. Notice that the flexibility index of nominal design is only 0.249. Let further assume that all revamp options are allowed in this case. From the values of the binary variables y_j, the active constraints are associated with $\overline{F}_{w1}^U$, $\overline{CI}_{u4}^U$, $\overline{CO}_{u1}^U$, $\overline{CO}_{u2}^U$, $\overline{CO}_{u3}^U$, and $\overline{CO}_{u4}^U$. According to the proposed heuristics, the last five of these active constraints may be relaxed with auxiliary pipelines. Let us first analyze these possibilities:

1. Constraints $\overline{CI}_{u4}^U$ and $\overline{CO}_{u4}^U$: Both constraints can be relaxed by increasing the throughput and/or lowering the inlet concentration of unit $u4$. These tasks can be achieved by sending a clean water flow to $u4$. According to Table 5, the output of unit $t1$ is clearly the best choice because its pollutant concentration is relatively low and, also, adding a stream from $t1$ to $u4$ will not affect other constraints. Therefore, we connect unit $t1$ to unit $u4$ as our first design option (design III-A). The optimal solution shows that the flexibility index of design III-A can only be raised to 0.280. This is due to the fact that, since the output of $u4$ is eventually directed to $t1$, the throughput limit of unit $t1$ prevent a large recycle flow from $t1$ to $u4$.
2. Constraint $\overline{CI}_{t1}^U$: This constraint may be relaxed by adding a self-recycling flow around unit $t1$ as the next design option (design III-B). From the optimal solution of the corresponding flexibility index model it can be observed that the flexibility index again can only reach 0.280. The reason for this is the same as that described for design III-A.
3. Constraint $\overline{CO}_{u1}^U$: Since the inlet concentration limit of $u1$ is very low, it is not possible to identify a water source in the given network which is clean enough for relaxing the constraint under consideration.
4. Constraints $\overline{CO}_{u2}^U$ and $\overline{CO}_{u3}^U$: These two constraints may be relaxed by diverting the outlet stream from $t1$ to $u2$ and $u3$ respectively to increase their throughputs. This action obviously will result in the same problem as that encountered in design III-A or III-B, namely, the throughput limit of unit $t1$. To confirm this prediction, the impacts of connecting unit $t1$ to unit $u2$ (design III-C) and connecting unit $t1$ to unit $u3$ (design III-D) have been evaluated. As expected, neither design III-C nor III-D can be adopted to improve the operational flexibility to a satisfactory level. In fact, the flexibility levels in both cases are the same as those achieved in design III-A and design III-B. Since each of the two options is individually hampered by the throughput limit of unit $u1$, the improvement should still be minimal if both changes are combined together in the next design option, design III-E. This prediction can be confirmed in the solution of the corresponding flexibility index model, as the flexibility index for this design is also 0.280.

In the next phase of the proposed revamp procedure, it is required to upgrade the existing treatment unit (design III-F). Let us assume that the removal ratio of unit $t1$ can be improved to 0.9. However, since the water flow from unit $t1$ is directed only to the sink in the nominal design, upgrading $t1$ only relaxes the concentration constraint at $s1$. As there are no changes in network structure, no improvement can be anticipated either. The solution of the corresponding model shows that the flexibility level of design III-F is not different from the original level (0.249). Therefore, it can be concluded that the operational flexibility of a water network cannot be enhanced by applying the design heuristics to improve a constraint which is originally not active (corresponding to $\overline{C}_{s1}^U$ in this particular case).

In the final revamp phase, the possibilities of installing additional treatment units are explored. Let us assume that the available new treatment units are of the same type and their removal ratios are the same (0.9). Following is a list of possible locations for these units.

1. Constraints $\overline{CI}_{u4}^U$ and $\overline{CO}_{u4}^U$: These two constraints can be relaxed simultaneously by placing the new treatment unit $t2$ before unit $u4$ to lower the pollutant concentration of the

secondary water and, also, diverting a portion of the outlet flow of unit $t2$ to sink $s1$. This option is referred to as design III-G in this paper (see Fig. 6). The solution of the corresponding model shows that this design is flexible enough, as the flexibility index can be improved to 1.604. The minimized operating cost can also be reduced to 282.383 $/h.

2. Constraints $\overline{CO}_{u1}^{U}$ and $\overline{CO}_{u2}^{U}$: As freshwater is used in $u1$ and $u2$, it makes no sense to install new treatment units to produce cleaner inputs for these units.
3. Constraint $\overline{CO}_{u3}^{U}$: This constraint can be relaxed by installing a new treatment unit $t2$ before $u3$ to lower the pollutant concentration of the secondary water source and again diverting a portion of the outlet flow of $t2$ to sink $s1$ (see design III-H in Fig. 7). The rationale for adopting this design is similar to that for design III-G. The solution of the corresponding flexibility index model shows that the operational flexibility of design III-H also reaches a satisfactory level of 1.314. The minimized operation cost can be reduced to 291.857 $/h.
4. Constraint $\overline{F}_{t1}^{U}$: Although this constraint is not active in the original nominal design, it becomes active in several revamped versions, i.e., III-A, III-B, III-C, III-D and III-E. We will try to improve design III-B by installing unit $t2$ to work in parallel with unit $t1$, hence relaxing its throughput limit (see design III-I in Fig. 8). The optimal solution shows that this design can also be adopted to adequately compensate the anticipated disturbances, as the flexibility index is raised to 1.071. The minimized operation cost can be reduced to 220.021 $/h.

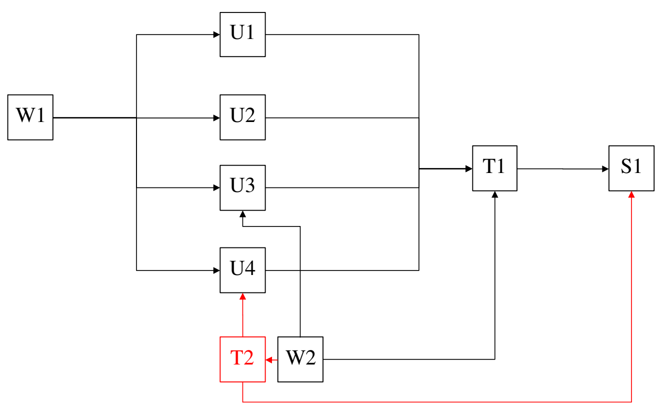

Fig. 6. Revamp design III-G.

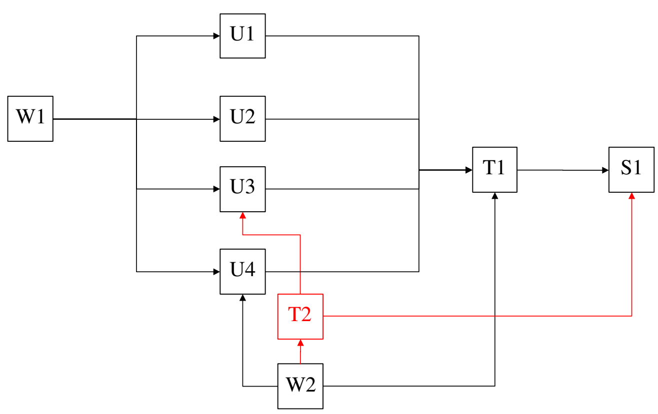

Fig. 7. Revamp design III-H.

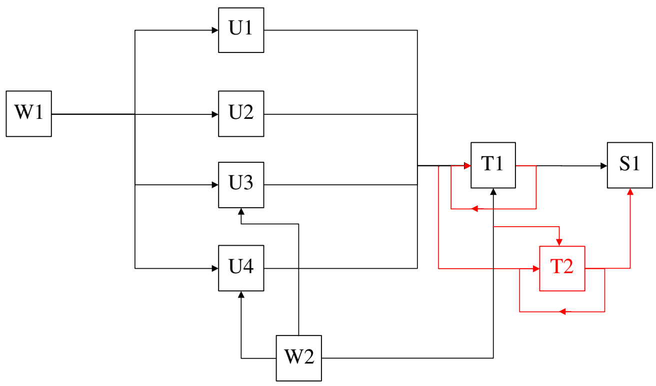

Fig. 8. Revamp design III-I.

Since more than one design, i.e., III-G, III-H and III-I, can be used to achieve the desired flexibility level, additional criteria must be adopted to select the most appropriate one for actual application. For example, if there is no room for unit $t2$ to work in parallel with unit $t1$ because the surrounding space is already very crowded, then design III-I should be excluded from consideration. Other than the practical concerns, the operating cost can also be used to facilitate decision making. Notice that the operating cost of design III-I is the lowest among the above three candidates. However, it should also be noted that this design requires the largest number of new pipelines. This means that we may also have to purchase more control equipments, as the flexibility index defined by Grossmann (1985a,b) is based on manipulating control variables to overcome disturbances. On the other hand, choosing between design III-G and III-H is easier because design III-G is superior to design III-H in terms of both flexibility and operating cost. Design III-G should therefore be selected over III-H if there are no other contradictory factors to be considered.

6. Conclusions

A novel heuristic strategy is developed in this work to improve the operation resiliency of any existing water network by relaxing the active constraints identified in the optimal solution of flexibility index model. Each of the proposed structural modifications, i.e., introducing the auxiliary pipelines, upgrading the existing treatment units, and installing new treatment units, may be used for this purpose when increasing the upper limit of freshwater supply rate is not effective or not possible. The appropriate revamp options can be selected systematically with the aid of proposed design heuristics. From the results obtained so far in case studies, it can be concluded that this simple heuristic approach can provide good starting points for a rigorous method and reasonably good designs in practical applications.

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