An algorithmic revamp strategy for improving operational flexibility of multi-contaminant water networks

Da Jiang \textsuperscript{a}, Chuei-Tin Chang \textsuperscript{b,}\textsuperscript{*}

\textsuperscript{a} Key Laboratory of Advanced Control and Optimization for Chemical Processes, East China University of Science and Technology, Ministry of Education, Shanghai 200237, P.R. China

\textsuperscript{b} Department of Chemical Engineering, National Cheng Kung University, 1 University Road, Tainan 70101, Taiwan, ROC

HIGHLIGHTS

- A programming based method is proposed for revamping water networks.
- A novel strategy is developed to ensure convergence of iterative FI calculation.
- The reliability of this strategy is shown with numerical experiments.
- The best revamp options are identified with a modified genetic algorithm.
- The effectiveness of this approach is demonstrated in case studies.

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ABSTRACT

The flexibility index (FI) has often been used in the past as one of the key performance measures of single-contaminant water network designs. The traditional approach to compute such an index is to solve a MINLP model derived according to the Karush–Kuhn–Tucker conditions. For the multi-contaminant systems, this approach may be impractical due to the overwhelming efforts required in deriving and solving the corresponding models. To overcome these difficulties, an alternative computation strategy is devised in this study to determine FI by solving a NLP model iteratively. On the basis of this modified computation method, the proper revamp options can be identified automatically with genetic algorithm. A series of case studies have also been carried out in this work to verify the feasibility and effectiveness of the proposed approach. In every example studied so far, the converged optimization results were not only satisfactory but also obtained within a reasonable period of time.

1. Introduction

Increasing public concern on the scarcity of water resources, together with stringent regulations on the waste water effluents, has prompted a great number of recent studies on water network designs. Various water management issues have already been addressed rigorously and several thorough reviews are available in the literature. For example, Bagajewicz (2000) conducted a survey with emphasis on the systematic optimization-based techniques; Foo (2009) focused on the “Pinch” methods; Gouws et al. (2010) presented an overview of the developments and methodologies proposed for batch water networks; Jezowski (2010) gave an analysis of the water network problem formulation and an extensive review of the solution techniques.

Notice first that most published works on water network synthesis were performed on the basis of fixed process conditions, e.g., see Huang et al. (1999), Tsai and Chang (2001), Gabrieland El-Halwagi (2005), Ponce-Ortega et al. (2009), Nápoles-Rivera et al. (2012) and Rubio-Castro et al. (2013). Since the total annual cost was usually adopted as the objective function in the conventional model, the resulting network configurations were inevitably quite complex so as to facilitate reuse-recycle and reuse-regeneration. These structures are bound to hamper efficient operation and control under the influences of uncertain disturbances from environment. Moreover, the highly integrated designs obtained on the basis of uncertain model parameters may even be infeasible in practice. For these reasons, Jezowski (2010) suggested that there is a need for designing flexible water networks.

In their pioneering work, Swaney and Grossmann (1985a,b) developed the definition of flexibility index (FI) for use as a quantitative measure of the feasible region in the space of uncertain parameters. The expected deviations of each parameter from its nominal value were assumed to be estimable in the positive and negative directions, while the corresponding actual deviations can be regarded as the products of the expected deviations and a common scalar variable.
Generally speaking, the index FI is associated with the maximum actual deviations, by which feasible operation can be guaranteed with proper manipulation of the control variables.

Originally FI was determined with the so-called vertex method (Halemane and Grossmann, 1983). Grossmann and Floudas (1987) later proposed an alternative solution strategy for a multi-level optimization problem according to the following ideas: (i) the inner optimization problem is replaced by the Karush–Kuhn–Tucker (KKT) optimality conditions; (ii) the discrete nature of the selection of the active constraints is utilized by introducing a set of binary variables to express if a specific constraint is active. Most flexibility index calculations in recent publications were performed with this approach, which has been referred to in the literature as the active set method. A few additional works also addressed the feasibility and flexibility issues in the non-convex problems (Floudas et al., 2001; Goyal and Ierapetritou, 2003; Banerjee and Ierapetritou, 2005; Tay et al., 2011).

On the basis of the aforementioned concept of flexibility index, Chang et al. (2009) developed a generalized mixed-integer nonlinear programming model for assessing and improving the operational flexibility of water network designs. They found that operational flexibility of any given network can be enhanced with two revamp strategies, i.e., (1) relaxation of the upper limit of freshwater supply rate and (2) installation of auxiliary pipelines and/or elimination of existing ones. Based on the insights gained from active constraints, Riyanto and Chang (2010) developed a heuristic revamp strategy in a subsequent study to improve the operational flexibility of existing water networks. Finally, Li and Chang (2011) developed a new nonlinear programming formulation model by incorporating process knowledge into the conventional vertex method to simplify FI calculation.

Although satisfactory results have been reported, it is still necessary to carry out further research on flexible network design because only the single-contaminant systems were considered in the above studies. The revamp heuristics used previously for flexibility enhancement may not be valid in the multi-contaminant applications and, more importantly, the total number of candidate configurations may be too large to be evaluated in a manual evolution procedure. Furthermore, if the active set method is to be utilized for FI calculation, the KKT conditions must be invoked to manually construct the flexibility index model for the multi-contaminant case and the required derivation can be very demanding. Finally, it is obvious that the iterative solution process of the above MINLP model for computing FI may not always converge. This inherent characteristic is really unacceptable if an automatic search strategy is to be implemented to identify the more flexible revamp designs.

To circumvent the drawbacks mentioned above, a number of novel solution techniques have been developed in this work to generate the desired structures. Specifically,

- To simplify the task of model construction and to ensure convergence in FI calculation, the single-vertex flexibility test (Li and Chang, 2011) is performed repeatedly in a bisection search procedure;
- To promote search efficiency and reliability, an improved genetic algorithm (GA) is adopted to identify proper revamp design(s) in an evolution procedure.

The remaining paper is organized as follows. The general framework of an augmented superstructure and the corresponding model constraints are described in detail in the following section. A simple search algorithm for computing the flexibility index of a given network is then proposed in Section 3. To validate this solution strategy, a series of numerical experiments have been performed. The optimization results of three examples are analyzed and reported in Section 4. The next section outlines the technical details in implementing the genetic algorithms for identifying the proper revamp design(s) among a large number of candidates. To demonstrate the effectiveness of this approach, the descriptions of three case studies are provided in Section 6. Finally, the concluding comments are given in the last section.

2. Augmented superstructure and its model constraints

Since it is very tedious and inefficient to construct different versions of the flexibility index model for various candidate designs and then carry out the needed optimization runs, a generalized model has been formulated and used in this work as a design tool for all possible structures under consideration. To develop such a model on the basis of an existing network, it is necessary to first build an augmented superstructure in which all possible new connections are embedded.

2.1. Label sets

For illustration convenience, let us first define the following label sets:

- $W_1 = \{w_1 | w_1 \text{ is the label of an existing primary water source}\}$
- $W_2 = \{w_2 | w_2 \text{ is the label of an existing secondary water source}\}$
- $S = \{s | s \text{ is the label of an existing sink}\}$
- $U = \{u | u \text{ is the label of an existing water using unit}\}$
- $T = \{t | t \text{ is the label of an existing treatment unit}\}$
- $X = \{x | x \text{ is the label of an added treatment unit}\}$
- $K = \{k | k \text{ is the label of a water contaminant}\}$

Based on the above definitions, one can then assemble the following sets for characterizing the superstructure:

- The label set of all water sources embedded in superstructure, i.e., $W = W_1 \cup W_2$
- The label set of all processing units embedded in superstructure, i.e., $P = U \cup T \cup X$
- The label set of all existing processing units, i.e., $P' = U \cup T$
- The label set of all split nodes in superstructure, i.e., $M = W \cup U \cup T \cup X$
- The label set of all split nodes at the outlets of existing units, i.e., $M' = W \cup U \cup T$
- The label set of all mixing nodes in superstructure, i.e., $N = U \cup T \cup X \cup S$
- The label set of all mixing nodes at the inlets of existing units, i.e., $N' = U \cup T \cup S$
2.2. Superstructure construction

A conventional superstructure for grassroots designs can be constructed according to the following steps:

(1) Connect the split node at the outlet of every primary water source in \( W_1 \) to the mixing node at the inlet of every processing unit in \( P \).
(2) Connect the split node at the outlet of every secondary water source in \( W_2 \) to every mixing node in \( N \).
(3) Connect the split node at the outlet of every processing unit in \( P \) to every mixing node in \( N \).

This conventional configuration can then be transformed into an augmented superstructure by classifying all embedded connections into three classes on the basis of existing connections and units in the given water network. More specifically, these connection types can be associated respectively with: (1) the existing pipelines, (2) the new pipelines between existing units, i.e., the connections from \( M' \) to \( N' \), which are not present in the given network, and (3) the new pipelines between the added treatment units and other units, i.e., the connections from \( M \) to \( X \) and from \( X \) to \( N \). Finally, to facilitate unambiguous formulation of the corresponding mathematical model, the notational convention in Table 1 is followed throughout this paper.

A simple example is given below to further clarify the above practices.

**Example 1.** Let us consider the existing water network presented in Fig. 1, in which a fresh water source \( (W_1) \), a water using unit \( (U_1) \), a wastewater treatment unit \( (T_1) \), and a sink \( (S_1) \) are involved. The corresponding augmented superstructure can be found in Fig. 2. The symbols \( F_{W_1}, F_{U_1}, F_{T_1}, \) and \( F_{S_1} \) in this superstructure respectively denote the throughputs in \( W_1, U_1, T_1 \), and \( S_1 \), while \( F_{W_1,U_1}, F_{U_1,S_1}, \) and \( F_{T_1,S_1} \) denote the flowrates in the existing pipelines (Type-1 connections), i.e., from \( W_1 \) to \( U_1 \), from \( U_1 \) to \( T_1 \), and from \( T_1 \) to \( S_1 \), respectively. Based on the classification criteria mentioned above, there can be four new pipelines connecting the split nodes in \( M' \) and the mixing nodes in \( N' \). Specifically, these Type-2 connections are: \((W_1, T_1), (U_1, S_1), (T_1, U_1), \) and \( (T_1, T_1) \), and the corresponding flow rates are expressed as \( f_{W_1,T_1}, f_{U_1,S_1}, f_{T_1,U_1}, \) and \( f_{T_1,T_1} \), respectively. If an extra treatment unit \( X_1 \) is allowed to be installed in this network, then at most six new pipelines may be added, i.e., \((W_1, X_1), (U_1, X_1), (T_1, X_1), (X_1, U_1), (X_1, T_1) \) and \( (X_1, S_1) \), and they should be regarded as Type-3 connections. Their flow rates are denoted respectively as \( f_{W_1,X_1}, f_{U_1,X_1}, f_{T_1,X_1}, f_{X_1,U_1}, f_{X_1,T_1}, \) and \( f_{X_1,S_1} \).

2.3. Model constraints

The equality and inequality constraints of the proposed mathematical programming model can be formulated on the basis of the augmented superstructure and the notational convention mentioned above. A brief summary is presented in the sequel:

- **Binary design parameters**
  In the proposed computation procedure, the flexibility index of a revamped network is calculated on the basis of the existing network and also a collection of new pipelines and/or new treatment units which are chosen from the outset. To facilitate model formulation, let us introduce the following binary design parameters:

\[
d_{m,n} = \begin{cases} 
1 & \text{if the new connection between } m \in M \text{ and } n \in N \text{ is chosen} \\
0 & \text{otherwise}
\end{cases}
\]

(1)

Note that these parameters should be fixed before computing the flexibility index. In addition, the following flow constraints should also be imposed:

\[
f^d_{m,n} \leq f_{m,n} \leq f^u_{m,n}
\]

(2)

- **Primary sources**
  The freshwater supplies secured by a chemical plant are regarded as the primary water sources in the model. It is also assumed that any effluent is not allowed to be mixed.

![Fig. 1. The existing water network in Example 1.](image-url)
with freshwater to meet the discharge limit required by environmental regulation. Mass balance at the outlet split node of every primary source can be written as

$$FT_{w_1} = \sum_{p \in P} F_{w_1, p} + \sum_{n \in P} F_{w_1, n}$$

(3)

In practical applications, an upper bound should be imposed upon the freshwater supply rate:

$$FT_{w_1} \leq FT_{w_1}^{\max}$$

(4)

where, \( w_1 \in W_1 \).

• Secondary sources
  The pollutant concentrations in secondary water are usually higher than those in the primary source. The mass balance at the outlet split node can be expressed as

$$FT_{w_2} = \sum_{p \in P} F_{w_2, p} + \sum_{s \in S} F_{w_2, s} + \sum_{n \in N} F_{w_2, n}$$

(5)

where, \( w_2 \in W_2 \).

• Sinks
  The wastewater can be discharged into the environment or other effluent treatment facilities. The mass-balance constraints at the inlet mixing node of each sink can be expressed as

$$FT_s = \sum_{p \in P} F_{p, s} + \sum_{w_2 \in W_2} F_{w_2, s} + \sum_{m \in M} F_{m, s}$$

(6)

$$FT_{s, k} = \sum_{p \in P} F_{p, s} C_{p, k} + \sum_{w_2 \in W_2} F_{w_2, s} C_{w_2, k} + \sum_{m \in M} F_{m, s} C_{m, k}$$

(7)

where, \( s \in S \) and \( k \in K \). Obviously, an upper bound should be imposed on every contaminant concentration at the sink to conform to the environmental regulations:

$$C_{s, k} \leq C_{s, k}^{\max}$$

(8)

• Water using units
  The mass balances for characterizing the water using units are given below:

$$FT_u \left( C_{u,k}^{\text{in}} - C_{u,k}^{\text{out}} \right) = ML_{u,k}$$

(9)

$$FT_u = \sum_{w \in W} F_{w,u} + \sum_{p \in P} F_{p,u} + \sum_{m \in M} F_{m,u}$$

$$= \sum_{p \in P} F_{w_1, p} + \sum_{s \in S} F_{w_2, s} + \sum_{n \in N} F_{w_2, n}$$

(10)

where, \( u \in U \) and \( k \in K \). The upper limits of \( C_{u,k}^{\text{in}} \) and \( C_{u,k}^{\text{out}} \) must also be imposed, i.e.,

$$C_{u,k}^{\text{in}} \leq C_{u,k}^{\text{in, max}}$$

(11)

$$C_{u,k}^{\text{out}} \leq C_{u,k}^{\text{out, max}}$$

(12)

• Water treatment units
  The following mass-balance constraints are adopted in this work to model the water treatment units:

$$C_{u,k}^{\text{in}} \left( 1 - R_{t,k} \right) = C_{u,k}^{\text{out}}$$

(13)

$$FT_t = \sum_{w \in W} F_{w,t} + \sum_{p \in P} F_{p,t} + \sum_{m \in M} F_{m,t}$$

$$= \sum_{p \in P} F_{w_1, p} + \sum_{s \in S} F_{w_2, s} + \sum_{n \in N} F_{w_2, n}$$

(14)

where \( t \in T \) and \( k \in K \). For every treatment unit, the inequality constraints are usually imposed upon the water throughput and the pollutant concentrations at the inlet, i.e.,

$$FT_t \leq FT_t^{\max}$$

(15)

$$C_{u,k}^{\text{in}} \leq C_{u,k}^{\text{in, max}}$$

(16)
• New treatment units

The model constraints for these new treatment units are essentially the same as those for the existing ones, i.e.,

\[ C^w_{t,k}(1-R_{x,k}) = C^{out}_{x,k} \] (17)

\[ ft_x = \sum_{m \in M} f_{m,x} = \sum_{n \in N} f_{x,n} \] (18)

\[ ft_x C^m_{t,k} = \sum_{m \in M} f_{m,x} C_{m,k} \] (19)

where \( x \in X \) and \( k \in K \). For every new treatment unit, the upper bounds of the throughput and the pollutant concentrations at the inlet must also be included in the model, i.e.,

\[ ft_x \leq ft_x^{\text{max}} \] (20)

\[ C_{t,x}^{\text{in}} \leq C_{t,x}^{\text{max}} \] (21)

2.4. Uncertain multipliers

Since the actual operating conditions may vary with time, the values of some model parameters can be uncertain. A water network designed solely on the basis of nominal conditions may not be flexible enough to cope with all possible changes during operation. In this work, the following uncertain multipliers are adopted to facilitate systematic flexibility analysis:

\[ FT_{w_1}^{\text{max}} = FT_{w_1}^{\text{max}} \theta_{T_{w_1}}^{\text{max}} \forall w_1 \in W_1 \] (22)

\[ FT_{w_2} = FT_{w_2} \theta_{T_{w_2}} \forall w_2 \in W_2 \] (23)

\[ C_{w_2,k} = C_{w_2,k} \theta_{C_{w_2,k}} \forall w_2 \in W_2 \forall k \in K \] (24)

\[ ML_{u,k} = ML_{u,k} \theta_{ML_{u,k}} \forall u \in U \forall k \in K \] (25)

\[ \text{C}^{\text{in},\text{max}}_{t,k} = \text{C}^{\text{in},\text{max}}_{t,k} \theta_{\text{C}^{\text{in},\text{max}}_{t,k}} \forall u \in U \forall k \in K \] (26)

\[ \text{C}^{\text{out},\text{max}}_{t,k} = \text{C}^{\text{out},\text{max}}_{t,k} \theta_{\text{C}^{\text{out},\text{max}}_{t,k}} \forall u \in U \forall k \in K \] (27)

\[ R_{t,k} = R_{t,k} \theta_{R_{t,k}} \forall t \in T \forall k \in K \] (28)

\[ FT_t^{\text{max}} = FT_t^{\text{max}} \theta_{FT_t^{\text{max}}} \forall t \in T \] (29)

\[ \text{C}^{\text{in},\text{max}}_{t,k} = \text{C}^{\text{in},\text{max}}_{t,k} \theta_{\text{C}^{\text{in},\text{max}}_{t,k}} \forall t \in T \forall k \in K \] (30)

\[ R_{t,k} = R_{t,k} \theta_{R_{t,k}} \forall x \in X \forall k \in K \] (31)

\[ ft_x^{\text{max}} = ft_x^{\text{max}} \theta_{ft_x^{\text{max}}} \forall x \in X \] (32)

\[ \text{C}^{\text{in},\text{max}}_{x,k} = \text{C}^{\text{in},\text{max}}_{x,k} \theta_{\text{C}^{\text{in},\text{max}}_{x,k}} \forall x \in X \forall k \in K \] (33)

where \( FT_{w_1}, FT_{w_2}, C_{w_2,k}, ML_{u,k}, \text{C}^{\text{in},\text{max}}_{t,k}, \text{C}^{\text{out},\text{max}}_{t,k}, R_{t,k}, FT_t^{\text{max}}, \text{C}^{\text{in},\text{max}}_{t,k}, \) \( R_{t,k}, \) and \( \text{C}^{\text{in},\text{max}}_{x,k} \) represent the nominal values of the uncertain parameters; \( \theta_{FT_{w_1}}, \theta_{FT_{w_2}}, \theta_{C_{w_2,k}}, \theta_{ML_{u,k}}, \theta_{\text{C}^{\text{in},\text{max}}_{t,k}}, \theta_{\text{C}^{\text{out},\text{max}}_{t,k}}, \theta_{R_{t,k}}, \theta_{FT_t^{\text{max}}}, \theta_{\text{C}^{\text{in},\text{max}}_{t,k}}, \theta_{R_{t,k}}, \) and \( \theta_{\text{C}^{\text{in},\text{max}}_{x,k}} \) are the corresponding uncertain multipliers. Note that the nominal value of every uncertain multiplier always equals 1.

3. A simple search algorithm for flexibility index

Although several thorough reviews of the available solution strategies can be found in the literature, e.g., see Biegler et al. [1997], the basic model framework is still outlined in the sequel for illustration clarity and completeness. Let us respectively express the equality and inequality constraints in the aforementioned model as:

\[ h_i(d, z, x, \theta) = 0 \quad \forall i \in I \] (34)

\[ g_j(d, z, x, \theta) \leq 0 \quad \forall j \in J \] (35)

where,

\[ I = \{i| i \text{ is the label of an equality constraint}\}; \]

\[ J = \{jj| jj \text{ is the label of an inequality constraint}\}; \]

In addition, \( d \) represents a vector in which all binary parameters in Eq. (1) are stored; \( z \) denotes the vector of adjustable control variables; \( x \) is the vector of state variables; \( \theta \) denotes the vector of uncertain parameters (or multipliers). The parameter space \( \Gamma(\delta) \) can be expressed as

\[ \Gamma(\delta) = \{\theta^U - \delta \Delta \theta^{-} \leq \theta \leq \theta^U + \delta \Delta \theta^{+}\} \] (36)

where, \( \Delta \theta^{+} \) and \( \Delta \theta^{-} \) denote the vectors of expected deviations in the positive and negative directions respectively; \( \delta \geq 0 \) is a scalar variable. The flexibility index \( F \) was traditionally regarded as the maximum value of \( \delta \) that renders all points in \( \Gamma(\delta) \) feasible. In previous studies, FL has usually been determined with the so-called active set method by solving a non-convex MINLP model (Grossmann and Floudas, 1987). Although this method is theoretically sound, there are a number of drawbacks for the present application. In particular, because of the need to invoke Karush–Kuhn–Tucker conditions, the resulting model is often tedious to construct even for a moderately complex water network. Another more serious disadvantage can be attributed to the fact that the convergence of optimization run cannot be guaranteed. This feature is unacceptable when, for the purpose of identifying the best revamp design in an evolutionary procedure, the aforementioned MINLP model must be solved repeatedly for various combinations of the binary parameters in \( d \).

To overcome the above difficulties, the flexibility index is computed in this study by solving the flexibility test problem iteratively according to the underlying principles of vertex method. Specifically, for a given value of scalar variable \( \delta \) and a given set of binary parameters \( d \), the feasibility of a water network design can be tested by carrying out the optimization run required by the following formulation:

\[ \chi(d) = \max_{k \in V} \min_{u \in \Delta} u \] s.t.

\[ h_i(d, z, x, \theta^U) = 0 \quad \forall i \in I \]

\[ g_j(d, z, x, \theta^U) \leq 0 \quad \forall j \in J \] (37)

where \( V \) denotes the set of all vertices in \( \Gamma(\delta) \) and \( \theta^U \) is one of them in this set (i.e., vertex \( k \)). The design is considered to be feasible if \( \chi(d) \geq 0 \), while infeasible if otherwise. It can also be observed from Eq. (37) that the minimum values of \( u \) at all vertexes must be determined in this optimization problem.

Due to the special model structure for water networks, Li and Chang (2011) suggested that the problem in Eq. (37) can in fact be simplified by checking only a single critical vertex. This critical point is associated with the upper or lower limit of each uncertain parameter on the basis of physical insights, i.e.,
the upper bounds of
• the pollutant concentrations at secondary sources and
• the mass loads of water using units, and
• the lower bounds of
• the estimated maximum freshwater supply rates
• the allowed maximum inlet and outlet pollutant concentrations of water using units
• the removal ratios of waste water treatment units
• the allowed maximum throughputs of treatment units and
• the allowed maximum inlet pollutant concentrations of treatment units.

Finally, note that the critical limit for the supply rate of every secondary source can only be identified on a case-by-case basis. If the secondary water is too dirty to be consumed by any water using unit, the upper bound of its flow rate should be treated as the limiting constraint. Otherwise, the lower bound must be chosen.

For the purpose of reducing computation load, the aforementioned single-vertex test is performed repeatedly to guide the search for determining the flexibility index \( F_l \). More specifically, the simple bisection strategy is adopted to locate the maximum feasible \( \delta \) on the basis of a set of given binary parameters in \( d \). Following is a description of the proposed search algorithm:

1. Let \( n=0 \). Set the lower bound of the flexibility index to be \( F_{l,\text{low}} = 0 \) and the upper bound \( F_{l,\text{up}} \) an arbitrarily selected large number.
2. Let \( \delta = \frac{F_{l,\text{up}} + F_{l,\text{low}}}{2} \) and perform the single-vertex flexibility test.
3. Let \( n = n + 1 \). If the test in Step 2 is feasible, set \( F_{l,\text{low}} = \delta \) and \( F_{l,\text{up}} = F_{l,\text{up}, -1} \). Otherwise, set \( F_{l,\text{low}} = F_{l,\text{low}, -1} \) and \( F_{l,\text{up}} = \delta \).
4. Check if a given termination criterion (say, \( F_{l,\text{up}} - F_{l,\text{low}} < \epsilon \)) is satisfied. If not, go to Step 2. Otherwise, stop.

Note that an implied assumption in the above procedure is that the test result for \( \delta = F_{l,\text{up}} \) is infeasible. If this is not the case with the selected initial guess, then the upper bound must be enlarged to satisfy this requirement.

4. Numerical experiments

Three examples are presented below to demonstrate the feasibility and superiority of the single-vertex search algorithm. All problems were solved on a PC, which is equipped with an Intel® Core™ i7 Quad CPU Q9400 and 4.00 GB RAM (3.25 GB usable) 32-bit operating system platform. The single-vertex flexibility test model was coded with GAMS and solved with BARON, while the bisection search procedure was realized using MATLAB via MATLAB-GAMS interface.

Example 2. Let us consider the nominal water network presented in Fig. 3, in which one freshwater source \((W_1)\), one secondary source \((W_2)\), three water using units \((U_1, U_2, \text{and } U_3)\), two waste-water treatment units \((T_1 \text{ and } T_2)\) and a sink are involved. The model parameters for this example are presented in Table 2. Six uncertain multipliers are considered in this example and their expected deviations are:

\[
\begin{align*}
\Delta \theta_{C_{W_1}}^{+} &= \Delta \theta_{C_{W_1}}^{-} = 0.1 \\
\Delta \theta_{C_{W_2}}^{+} &= \Delta \theta_{C_{W_2}}^{-} = \Delta \theta_{C_{W_3}}^{+} = \Delta \theta_{C_{W_3}}^{-} = \Delta \theta_{C_{T_1}}^{+} = \Delta \theta_{C_{T_1}}^{-} = 0.15 \\
\Delta \theta_{C_{T_2}}^{+} &= \Delta \theta_{C_{T_2}}^{-} = \Delta \theta_{C_{S_1}}^{+} = \Delta \theta_{C_{S_1}}^{-} = 0.03
\end{align*}
\]

Note also that this example is taken from Riyanto and Chang (2010), and the flexibility index was found to be 0.32 with the active set method.

The convergence process of bisection search with the single-vertex method is described in Fig. 4. Notice that both the upper and lower bounds if \( F_l \) are plotted at every iteration, and their initial guesses were set to be 16 and 0, respectively. It is clear that the search converges after about 10 iterations to the correct value. The computation time in this case is 152 s, while a much longer 571 s is needed if the traditional vertex method is used to perform the flexibility test.

Example 3. Since the aforementioned single-vertex strategy has only been applied to the single-contaminant systems in the past (Li and Chang, 2011), it is obviously desirable to extend it to the multi-contaminant applications. For this purpose, let us consider the nominal water network presented in Fig. 5 and the corresponding model parameters in Table 3. In this example, let us assume that there are only four uncertain multipliers and their expected deviations are:

\[
\begin{align*}
\Delta \theta_{C_{W_1}}^{+} &= \Delta \theta_{C_{W_2}}^{-} = \Delta \theta_{C_{W_3}}^{+} = \Delta \theta_{C_{W_3}}^{-} = 0.1
\end{align*}
\]

Note also that this example is taken from Riyanto and Chang (2010), and the flexibility index was found to be 0.32 with the active set method.

The convergence process of bisection search with the single-vertex method is described in Fig. 4. Notice that both the upper and lower bounds if \( F_l \) are plotted at every iteration, and their initial guesses were set to be 16 and 0, respectively. It is clear that the search converges after about 10 iterations to the correct value. The computation time in this case is 152 s, while a much longer 571 s is needed if the traditional vertex method is used to perform the flexibility test.

Example 3. Since the aforementioned single-vertex strategy has only been applied to the single-contaminant systems in the past (Li and Chang, 2011), it is obviously desirable to extend it to the multi-contaminant applications. For this purpose, let us consider the nominal water network presented in Fig. 5 and the corresponding model parameters in Table 3. In this example, let us assume that there are only four uncertain multipliers and their expected deviations are:

\[
\begin{align*}
\Delta \theta_{C_{W_1}}^{+} &= \Delta \theta_{C_{W_2}}^{-} = \Delta \theta_{C_{W_3}}^{+} = \Delta \theta_{C_{W_3}}^{-} = 0.1
\end{align*}
\]

Table 2. The model parameters used in Example 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_{W_1}^{\text{max}} )</td>
<td>30.0</td>
<td>( C_{W_1}^{\text{max}} )</td>
<td>200.0</td>
</tr>
<tr>
<td>( C_{W_1} )</td>
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<td>( C_{W_2}^{\text{max}} )</td>
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</tr>
<tr>
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<tr>
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<td>( M_{W_1}^{\text{max}} )</td>
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</tr>
<tr>
<td>( C_{W_5} )</td>
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<td>( M_{W_2}^{\text{max}} )</td>
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</tr>
<tr>
<td>( C_{W_6} )</td>
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<td>( M_{W_3}^{\text{max}} )</td>
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</tr>
<tr>
<td>( C_{W_7} )</td>
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<td>( M_{W_4}^{\text{max}} )</td>
<td>0.9</td>
</tr>
<tr>
<td>( C_{W_8} )</td>
<td>50.0</td>
<td>( M_{W_5}^{\text{max}} )</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Fig. 3. The nominal structure of water network in Example 2.
The model parameters used in Example 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F^\text{max}_{w1}$</td>
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<td>(ppm)</td>
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<tr>
<td>$F_{w1}$</td>
<td>(t/h) 30.0</td>
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<td>(ppm)</td>
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<td>$C^\text{max}_{w1,B}$</td>
<td>(ppm)</td>
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<tr>
<td>$C_{w1,B}$</td>
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<td>$C^\text{max}_{w1,B}$</td>
<td>(ppm)</td>
</tr>
<tr>
<td>$C^\text{max}_{w1,A}$</td>
<td>(ppm) 10.0</td>
<td>$C^\text{max}_{w1,B}$</td>
<td>(ppm)</td>
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<tr>
<td>$C^\text{max}_{w1,B}$</td>
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<td>$C^\text{max}_{w1,B}$</td>
<td>(ppm)</td>
</tr>
<tr>
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<td>(ppm)</td>
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<td>$R_{U1,A}$</td>
<td>(kg/h)</td>
</tr>
<tr>
<td>$C^\text{max}_{w1,B}$</td>
<td>(ppm) 185.0</td>
<td>$R_{U1,B}$</td>
<td>(kg/h)</td>
</tr>
</tbody>
</table>

$\Delta \theta^+_{\text{MLu}_{4,2}} = \Delta \theta^+_{\text{MLu}_{1,2}} = 0.2$

$\Delta \theta^+_{\text{MLu}_{1,2}} = \Delta \theta^+_{\text{MLu}_{1,3}} = 0.3$

The flexibility index of this network can be found to be 0.491 by the traditional active set method.

Although the critical vertex can be determined according to the selection criteria described in the previous section, i.e., the corner point corresponding to the upper bounds of all mass loads in the present example, each vertex has been tested in the proposed bisection search procedure to produce a corresponding “flexibility index.” The results of 16 separate runs can be found in Table 4. It can be clearly observed that the correct IV value can indeed be obtained with the proposed single-vertex approach.

### Example 4

The last example in this section is adopted to demonstrate the advantage of the proposed computation strategy for solving large problems. Let us consider the complex nominal water network presented in Fig. 5, in which three (3) contaminants, one freshwater source ($W_1$), one secondary source ($W_2$), four water using units ($U_1$, $U_2$, $U_3$, $U_4$), a wastewater treatment units ($T_1$), and a sink ($S_1$) are involved. The corresponding model parameters are presented in Table 5. It is also assumed that there are 18 uncertain multipliers and the corresponding expected deviations are:

- $\Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{1,4}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{2,4}} = \Delta \theta^+_{\text{MLu}_{4,3}} = \Delta \theta^+_{\text{MLu}_{4,4}} = 0.15$

- $\Delta \theta^+_{\text{MLu}_{1,2}} = \Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{2,2}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{3,2}} = \Delta \theta^+_{\text{MLu}_{3,3}} = 0.25$

- $\Delta \theta^+_{\text{MLu}_{1,4}} = \Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{2,4}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{3,4}} = \Delta \theta^+_{\text{MLu}_{3,3}} = 0.2$

- $\Delta \theta^+_{\text{MLu}_{4,2}} = \Delta \theta^+_{\text{MLu}_{1,4}} = \Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{2,4}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{3,4}} = \Delta \theta^+_{\text{MLu}_{3,3}} = 0.3$

- $\Delta \theta^+_{\text{MLu}_{4,4}} = \Delta \theta^+_{\text{MLu}_{1,4}} = \Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{2,4}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{3,4}} = \Delta \theta^+_{\text{MLu}_{3,3}} = 0.1$

- $\Delta \theta^+_{\text{MLu}_{4,4}} = \Delta \theta^+_{\text{MLu}_{1,4}} = \Delta \theta^+_{\text{MLu}_{1,3}} = \Delta \theta^+_{\text{MLu}_{2,4}} = \Delta \theta^+_{\text{MLu}_{2,3}} = \Delta \theta^+_{\text{MLu}_{3,4}} = 0.05$

A problem of this scale cannot really be solved with the active set method in a reasonable time period (say, 24 h). However, it took only 18 s for the proposed search to converge and a flexibility index of 0.0165 was found for the given system.
to identify proper revamp designs for improving the operational flexibility of the revamped system, while FM$_2$ can be viewed as a cost-penalized version of FM$_1$.

The “fittest” individual(s) is obviously associated with one with the largest measure. The GA Toolbox v1.2 in MATLAB ([Chipperfield et al., 1994] is used to facilitate the required evolutionary computation procedure. Basically four standard evolutionary steps are performed for each generation, i.e., selection, recombination, mutation and reinsertion.

In all cases presented in this paper, the same GA parameters have been utilized in every run. A brief summary is given below:

- The population size was always set to be 100.
- The generation gap in the selection step was chosen to be 0.7.
- The crossover rate in the recombination step was 0.7.
- The mutation probability was fixed at the default value of 0.7/Lind in the mutation step, where Lind is the chromosome length.
- In the reinsertion step, the offspring individuals were ranked according to their fitness measures and top 50% of them were selected to replace the same number of least-fit parents.

The evolutionary procedure was terminated if (1) the total number of evaluated generations exceeded 200 and, also, (2) the largest fitness measure in a population stayed approximately the same for at least 30 generations.

Finally, since each FI is determined iteratively and this computation process can be very time-consuming, an additional mechanism has been built into the MATLAB code to avoid repeating the same calculation for identical network configurations. In particular, the individuals and their corresponding fitness measures in the parent generation and those in all previous generations can be accumulated in a data base. Every newly created individual in the offspring generation can be compared with the ones already stored there. If a match is identified, the corresponding fitness measure can be directly retrieved without the iterative computation.

### 5. Identification of revamp designs

As mentioned previously, the ultimate objective of this work is to identify proper revamp designs for improving the operational flexibility of any given water network. The allowed revamp options are limited to those incorporated in the augmented superstructure, i.e., the new pipelines and/or treatment units. The specifications of embedded treatment units are assumed to be available in advance. Since the number of alternative structures increases exponentially with the network complexity, a deterministic search strategy may fail to identify the optimal solution within a reasonable period of time. Therefore, a modified version of genetic algorithm (GA) has been adopted to circumvent this drawback. Notice also that, in a typical GA evolution procedure, every chromosome in a population can be expressed as a string of 0’s and 1’s, and this mechanism can be easily utilized for coding the structural optimization problem considered here.

In the proposed algorithm, the binary parameters defined in Eq. (1), i.e., the elements of vector $d$ in Eqs. (34) and (35), are encoded in every individual within a population. Essentially two alternative fitness measures (FM) can be considered for the purpose of generating revamp designs, i.e.,

\[
FM_1 = FI \tag{38}
\]

or

\[
FM_2 = \frac{\text{Fl}}{\sum d_{m,n}} \tag{39}
\]

Note that the flexibility index $FI$ in Eqs. (38) and (39) can be computed according to the single-vertex search algorithm described in Sections 3 and 4. In particular, FM$_1$ is a measure of the operational flexibility of the revamped system, while FM$_2$ can be viewed as a cost-penalized version of FM$_1$.

### 6. Case studies

The aforementioned evolution strategy has been tested extensively in a series of case studies. Three of them are summarized below:

#### 6.1. Case 1

Let us consider the nominal water network in Fig. 5 and the corresponding model parameters in Table 3. The uncertain parameters are the same as those described in Example 3. Without adding water treatment units, there are 11 new connections in the augmented superstructure. Additional treatment units could drastically increase the number of new connections in superstructure. For example, this number is raised from 11 to 32 if two new treatment units are allowed.

By using FM$_1$ as the fitness measure, more than one network structure was identified with the GA based method. It was observed that two new connections, i.e., ($T_1$, $U_1$) and ($T_1$, $U_2$), were embedded in all revamp options and, in fact, the highest FI value ($= 2.6953$) could also be achieved with these two indispensable additions only (see Fig. 7). On the other hand, the second fitness measure was also adopted in an additional GA run to address the need to limit piping cost in revamp designs. In fact, exactly one new pipeline ($T_1$, $U_2$) was called for in the optimum solution obtained with FM$_2$ (see Fig. 8). Notice that, although the flexibility index of this structure was slightly decreased to 2.3828, the piping cost was obviously also lower than that of Fig. 7. Finally, it was found that, although adding the aforementioned new pipeline(s) is
In their original work and the expected deviations were adopted:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{max}}$</td>
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<td>$C_{\text{out},\text{max}}$</td>
<td>(ppm) 200.0</td>
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<td>$W_{\text{w},\text{A}}$</td>
<td>(kg/h) 0.1</td>
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<td>$W_{\text{w},\text{A}}$</td>
<td>(kg/h) 2.0</td>
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<td>$W_{\text{w},\text{A}}$</td>
<td>(kg/h) 5.0</td>
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<td>25.0</td>
<td>$W_{\text{w},\text{A}}$</td>
<td>(kg/h) 7.0</td>
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<tr>
<td>$C_{\text{w},\text{A}}$</td>
<td>100.0</td>
<td>$R_{\text{w},\text{A}}$</td>
<td>(ppm) 0.8</td>
</tr>
</tbody>
</table>

The flexibility index of this original network was found to be 0.249 with the active set method.

Without incorporating any additional treatment unit, the number of new connections in the augmented superstructure can be found to be 25. The same FI value, i.e., 0.6445, was obtained by using either FM1 or FM2 in the GA evolution procedure. Three optimal structures were generated in the latter case (see Fig. 9) and each contains two new connections. Specifically, the added pipelines in these three designs are: (a) $(U_4, S_1)$ and $(T_1, U_2)$; (b) $(U_4, S_1)$ and $(T_1, U_3)$; (c) $(U_4, S_1)$ and $(T_1, U_4)$.

If one additional wastewater treatment unit $(X_4)$ (with a removal ratio of 0.9) is allowed to be added in the existing water network, 39 new connections are present in the augmented superstructure. It is obviously impractical to evaluate all $2^{39}$ possible structures. By following the proposed GA evolution procedure with either FM1 or FM2 as the fitness measure, the maximum FI was raised to the same value of 6.660. Only one solution was produced by using the latter measure (see Fig. 10), and this revamped design requires 4 new connections, i.e., $(T_1, U_2)$, $(U_4, X_1)$, $(X_1, U_1)$ and $(X_1, U_4)$. In this case, $\text{FM}_2 = 6.660/4 = 1.665$.

It should be noted that the highest FI value reported by Riyanto and Chang (2010) was only 1.604 for the present example. The corresponding revamp design consists of one new treatment unit (with a removal ratio of 0.9) and three new connections, i.e., $(U_4, X_1)$,
Thus, it can be observed from the values of both FI and FM2 that the flexibility index was reduced to 0.859 with the proposed programming based revamp strategy clearly outperforms the heuristic approach in this case study.

In this last case, let us consider the nominal structure described in Example 4. Note that this is the largest problem presented in the present paper.

The first scenario is concerned with an augmented superstructure in which additional the wastewater treatment units are not allowed. Thus, the total number of new connections should be 25. A maximum FI value of 1.331 was obtained by using FM1 as the fitness measure. On the other hand, the flexibility index was reduced to 0.859 with the second fitness measure FM2. Two alternative structures were obtained (see Fig. 11) and only one new pipeline was needed in each design, i.e., (a) \((T_4, U_1)\) and (b) \((U_1, U_4)\).

If two additional treatment units (with the same removal ratio of 0.9 for all contaminants) are allowed in the augmented superstructure, the total number of new connections should be increased to 53. Again FM1 and FM2 were used as the fitness measures in two separate GA runs. The resulting FI values were determined to be 3.332 and 3.327, respectively. The required computation time for the former run was 15,385 s, while that for the latter was 13,920 s. Finally, it was found that, by maximizing the second fitness measure, one new treatment unit \((X_2)\) and three new pipelines, i.e., \((U_4, X_2)\), \((X_2, U_3)\) and \((X_2, U_4)\), were selected in the optimal revamp design (see Fig. 12).

7. Conclusions

A programming based approach has been developed in this study to revamp any given water network for the purpose of flexibility enhancement. In order to alleviate the overwhelming manual and computational efforts required in deriving and solving the conventional flexibility index model with the active set method, a simple strategy is devised in this study to determine FI by repeatedly performing the flexibility test in a bisection search procedure. By incorporating this solution technique in genetic algorithm, more flexible revamp designs can be identified automatically on the basis of two alternative fitness measures. A series of numerical experiments and case studies have been carried out in this work to verify the feasibility and effectiveness of the proposed approach. In every example studied so far, the converged optimization results were not only satisfactory but also obtained within a reasonable period of time.

Nomenclature

\[
\begin{align*}
C_{m,k} & \quad \text{the concentration of contaminant } k \text{ at the outlet of unit } m \\
C_{s,k} & \quad \text{the concentration of contaminant } k \text{ at the outlet of unit } s \\
C_{p,k} & \quad \text{the concentration of contaminant } k \text{ in the secondary water from source } w_2 \\
C_{w_2,k}^{\text{in}} & \quad \text{the upper concentration limit of pollutant } k \text{ at the inlet of unit } t \\
C_{w_2,k}^{\text{in}, \text{max}} & \quad \text{the upper concentration limit of pollutant } k \text{ at the inlet of unit } x \\
C_{w_2,k}^{\text{max}} & \quad \text{the upper concentration limit of contaminant } k \text{ at the inlet of unit } t \\
C_{w_2,k}^{\text{out}, \text{max}} & \quad \text{the upper concentration limit of contaminant } k \text{ at the outlet of unit } u \\
C_{w_2,k}^{\text{out}} & \quad \text{the concentration of contaminant } k \text{ at the outlet of unit } u \\
\end{align*}
\]
the concentration of contaminant $k$ at the inlet of unit $x$
the concentration of contaminant $k$ at the outlet of unit $u$
the concentration of contaminant $k$ at the outlet of unit $t$
the concentration of contaminant $k$ at the outlet of unit $x$
the water flow rate in a new connection between split node $m$ and mixing node $n$

\[ F_{w,m,n} \]

the water flow rate in a new connection between source $w_1$ and unit $n$

\[ F_{w_1,n} \]

the water flow rate in a new connection between source $w_2$ and unit $n$

\[ F_{w_2,n} \]

the water flow rate in a new connection between unit $m$ and sink $n$

\[ F_{m,n} \]

the water flow rate in a new connection between unit $u$ and unit $n$

\[ F_{u,n} \]

the water flow rate in a new connection between unit $m$ and unit $u$

\[ F_{m,u} \]

the lower bound of water flow rate in a new connection

\[ F_{l} \]

the upper bound of water flow rate in a new connection

\[ F_{u} \]

the maximum throughput in new treatment unit $x$

\[ F_{w_1,p} \]

the water flow rate in existing connection between source $w_1$ and unit $p$

\[ F_{w_1,p} \]

the water flow rate in existing connection between source $w_2$ and sink $s$

\[ F_{w_2,s} \]

the water flow rate in existing connection between source $w_2$ and sink $s$

\[ F_{w_2,s} \]

the water flow rate in existing connection between unit $p$ and sink $s$

\[ F_{w_2,s} \]

the water flow rate in existing connection between source $w$ and sink $s$

\[ F_{w,s} \]

the water flow rate in existing connection between source $w$ and unit $u$

\[ F_{w,u} \]

the water flow rate in existing connection between unit $p$ and unit $u$

\[ F_{w,u} \]

the water flow rate in existing connection between unit $u$ and sink $s$

\[ F_{u,s} \]

the water flow rate in existing connection between unit $u$ and sink $s$

\[ F_{u,s} \]

the water supply rate from primary source $w_1$

\[ F_{TS,w_1} \]

the water supply rate from secondary source $w_2$

\[ F_{TS,w_2} \]

the water throughput in existing water-using unit $u$

\[ F_{TS} \]

the total water flow rate discharged to sink $s$

\[ F_{TS} \]

the water throughput in existing treatment unit $t$

\[ F_{TS} \]

the upper bound of water throughput in existing treatment unit $t$

\[ F_{TS} \]

the upper bound of freshwater supply rate from source $w_1$

\[ F_{TS} \]

the mass load of contaminant $k$ in unit $u$

\[ ML_{w,k} \]

the removal ratio of contaminant $k$ in unit $u$

\[ R_{k,u} \]

the removal ratio of contaminant $k$ in new treatment unit $x$

\[ R_{k,x} \]

References


