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

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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.

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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 water 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:

$$W_1 = \{w_1 | w_1 \textit{ is the label of an } \text{existing } \textit{primary water source}\}$$

$$W_2 = \{w_2 | w_2 \textit{ is the label of an } \text{existing } \textit{secondary water source}\}$$

$$S = \{s | s \textit{ is the label of an } \text{existing sink}\}$$

$$U = \{u | u \textit{ is the label of an } \text{existing } \textit{water using unit}\}$$

$$T = \{t | t \textit{ is the label of an } \text{existing } \textit{treatment unit}\}$$

$$X = \{x | x \textit{ is the label of an added } \text{treatment } \textit{unit}\}$$

$$K = \{k | k \textit{ is the label of a } \text{water contaminant}\}$$

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.,
  $N' = U \cup T \cup S$