# A Simple and Efficient Initialization Strategy for Optimizing Water-Using Network Designs

**Bao-Hong Li***

*Department of Chemical Engineering, Dalian Nationalities University, Dalian 116600, China*

**Chuei-Tin Chang**

*Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan 70101, Republic of China*

An efficient initialization strategy is developed in this work to solve the NLP and MINLP models for synthesizing water-using networks with multiple contaminants. A fairly good estimate of the optimal solution can be generated for any given problem according to a simple calculation procedure. Two published examples are adopted to demonstrate the effectiveness of the proposed approach. The optimum solutions obtained in this study are at least as good as those reported in the literature, while the computation time required to achieve convergence is significantly less.

## Introduction

Water is consumed in very large quantity in the chemical and petrochemical industries. In recent years, the severe shortages in freshwater resources and strict governmental regulations on industrial effluents have created strong incentives for water conservation. Takama et al.[1] first developed a mathematical program for optimal water allocation in a petroleum refinery based on a superstructure, in which all possible reuse and regeneration opportunities are embedded. Later, the so-called pinch method was proposed by Wang and Smith[2,3] to design water-using and wastewater-treatment networks separately. These pioneering works stimulated a series of enthusiastic research activities.[4−6] Notice that, to avoid handling the complex interactions between a water-using network and wastewater treatment network, most studies only focused on the design issues concerning either one of these two subsystems.

It has been well recognized that the pinch method is very helpful for understanding the intrinsic nature of a water-using network. In addition, the necessary theorem proposed by Bagajewicz and Savelski[7,8] is another useful tool for this purpose. In general, the single-contaminant water networks can be optimized routinely with available methods.[2,9] As for the multicontaminant case, the pinch method is really not applicable. The existing design approaches can be classified into two types. One of them can be regarded as a sequential procedure;[5,10] that is, the design of a water-using network is decomposed into a series of simpler steps and an acceptable solution can be obtained gradually. The other is referred to as the simultaneous method, in which a tree search strategy[11] or a superstructure-based mathematical program[12,13] is adopted to identify the optimal networks. Obviously, the solutions obtained with the sequential approach are usually suboptimal. On the other hand, the drawbacks of simultaneous optimization strategy are mainly due to the computation difficulties encountered in locating the global optimum.

Notice that the initial guesses adopted in solving an NLP or MINLP model always exerts a profound impact on the convergence process. Other than Chang and Li,[13] the initialization issues in synthesizing the optimal water networks have often been neglected in the past. In this paper, a simple and efficient strategy has been developed to generate near-feasible initial guesses for solving the NLP or MINLP problems needed for water network synthesis. The remaining paper is organized as follows. The problem statement and superstructure are provided in the next section. The mathematical programming model is then formulated, and the method to generate reliable initial guesses is explained in detail. At the end of this paper, the effectiveness of our proposed model and initialization method are demonstrated with two published examples. The solutions obtained with the proposed approach are at least as good as those reported in the literature, while a significant amount of computation time is saved in the convergence process.

## Problem Statement and Superstructure

According to Bagajewicz et al.,[11] the synthesis problem of a water-using network can be described as follows: "Given a set of water-using units in which multiple contaminants are involved, it is desired to determine a network of interconnections of water streams among the units so that the overall fresh water consumption is minimized while the units receive water of adequate quality."

To facilitate model formulation to solve the above problem, it is necessary to build a superstructure to incorporate all possible flow configurations. A substructure of that suggested by Chang and Li[13] is adopted in the present work (see Figure 1). Following is its construction procedure: (1) Place a mixing node at the inlet of every water-using unit. (2) Place a mixing node before the wastewater sink. (3) Place a splitting node after the freshwater source; the split branches from this node are connected to all the mixing nodes established in step 1. (4) Place a splitting node at the exit of every water-using unit. The split branches from every such node are connected to all the mixing nodes installed in steps 1 and 2 except the one before itself; that is, self-recycle is not allowed.

It should be noted that the self-recycle structure around every water-using unit is forbidden in this superstructure because such practice cannot promote water conservation.

* To whom correspondence should be addressed, Tel: 86-411-81633018. Fax: 86-411-87656217. E-mail: libh@dlnu.edu.cn.

10.1021/ie070702y CCC: $37.00 
Published on Web 11/08/2007

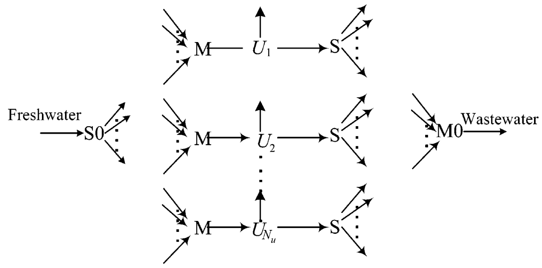


**Figure 1.** Generalized superstructure for water-using network.

## Mathematical Programming Model

To describe the mathematical programming model accurately, let us first introduce the definitions of two sets, i.e.: $\mathbf{U} = \{u \mid u$ is the label of a water-using unit; $u = 1, 2, ..., N_\mathrm{U}\}$; $\mathbf{K} = \{k \mid k$ is the label of a contaminant that affects the water quality; $k = 1, 2, ..., N_\mathrm{K}\}$.

The design objective can be expressed as

$$\mathrm{Min}\ f_\mathrm{T}^\mathrm{FW} \tag{1}$$

where $f_\mathrm{T}^\mathrm{FW}$ is the total freshwater consumption rate of the water-using network. It is subjected to the following constraints:

(1) At the source splitting node, the flow balance can be written as

$$f_\mathrm{T}^\mathrm{FW} = \sum_{u=1}^{N_\mathrm{U}} f_\mathrm{u}^\mathrm{FW} \tag{2}$$

where $f_\mathrm{u}^\mathrm{FW}$ is the freshwater consumption rate of water-using unit $u$.

(2) At the mixing node before water-using unit $u$, the water balance equation is

$$f_\mathrm{u}^{in} = f_\mathrm{u}^\mathrm{FW} + \sum_{u1=1,u1\neq u}^{N_\mathrm{U}} f_\mathrm{u1,u} \quad u,u1 \in \mathbf{U} \tag{3}$$

where $f_\mathrm{u1,u}$ represents the branch flow rate from water-using unit *u1* to $u$ and $f_\mathrm{u}^\mathrm{in}$ is the total flow rate after mixing node of unit $u$. In addition, the mass balances of contaminants should be

$$f_\mathrm{u}^\mathrm{in} c_\mathrm{u,k}^\mathrm{in} = \sum_{u1=1,u1\neq u}^{N_\mathrm{U}} f_\mathrm{u1,u} c_\mathrm{u1,k}^\mathrm{out} \quad u,u1 \in \mathbf{U}, k \in \mathbf{K} \tag{4}$$

where $c_\mathrm{u,k}^\mathrm{in}$ and $c_\mathrm{u,k}^\mathrm{out}$ are the concentrations of contaminant $k$ at the inlet of unit $u$ (after the mixing node) and the outlet of unit *u1* (before the splitting node) respectively.

(3) Around a water-using unit, the water and contaminant balances are

$$f_\mathrm{u}^\mathrm{in} = f_\mathrm{u}^\mathrm{out} + F_\mathrm{u}^\mathrm{L} \quad u \in \mathbf{U} \tag{5}$$

$$f_\mathrm{u}^\mathrm{in} c_\mathrm{u,k}^\mathrm{in} + M_\mathrm{u,k} = f_\mathrm{u}^\mathrm{out} c_\mathrm{u,k}^\mathrm{out} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{6}$$

where $F_\mathrm{u}^\mathrm{L}$ is the rate of water loss in unit $u$ and $M_\mathrm{u,k}$ is the mass load of contaminant $k$ to be removed in unit $u$.

(4) At the splitting node after each water-using unit, the flowrate balance is

$$f_\mathrm{u}^\mathrm{out} = \sum_{u1=1,u1\neq u}^{N_\mathrm{u}} f_\mathrm{u,u1} + f_\mathrm{u}^\mathrm{WW} \quad u,u1 \in \mathbf{U} \tag{7}$$

where $f_\mathrm{u}^\mathrm{WW}$ is the flow rate of wastewater generated by water-using unit $u$.

(5) Upper inlet and outlet concentration limits,

$$c_\mathrm{u,k}^\mathrm{in} \leq C\mathrm{in}_\mathrm{u,k}^\mathrm{max} \quad c_\mathrm{u,k}^\mathrm{out} \leq C\mathrm{out}_\mathrm{u,k}^\mathrm{max} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{8}$$

where $C\mathrm{in}_\mathrm{u,k}^\mathrm{max}$ and $C\mathrm{out}_\mathrm{u,k}^\mathrm{max}$ denote the maximum allowable concentrations of contaminant $k$ at inlet and outlet of unit $u$ respectively.

(6) Structural constraints. To manipulate structural complexity of the network, the maximum number of branch streams entering a mixing node or leaving a splitting node can be specified with the following constraints.

$$\sum_{u1=1,u1\neq u}^{N_\mathrm{U}} n_\mathrm{u1,u} + n_\mathrm{u}^\mathrm{FW} \leq NM_\mathrm{u}^\mathrm{max} \quad u,u1 \in \mathbf{U} \tag{9}$$

$$\sum_{u1=1,u1\neq u}^{N_\mathrm{U}} n_\mathrm{u,u1} + n_\mathrm{u}^\mathrm{WW} \leq NS_\mathrm{u}^\mathrm{max} \quad u,u1 \in \mathbf{U} \tag{10}$$

where, $n_\mathrm{u,u1}$ and $n_\mathrm{u1,u}$ are binary variables used to signify respectively whether the branches from unit $u$ to $u1$ and vice versa exist; $n_\mathrm{u}^\mathrm{FW}$ and $n_\mathrm{u}^\mathrm{WW}$ are binary variables associated with the branch streams from source to unit $u$ and from unit $u$ to sink, respectively; $NM_\mathrm{u}^\mathrm{max}$ and $NS_\mathrm{u}^\mathrm{max}$ represent the maximum branch numbers allowed to enter the mixing node and to leave the splitting node of unit $u$, respectively. To relate these binary variables to the corresponding flow rates, the following constraints are needed:

$$f_\mathrm{u,u1} \leq n_\mathrm{u,u1} F_\mathrm{u,u1}^\mathrm{max} \quad u,u1 \in \mathbf{U} \tag{11}$$

$$f_\mathrm{u}^\mathrm{FW} \leq n_\mathrm{u}^\mathrm{FW} \mathrm{FW}_\mathrm{u}^\mathrm{max} \quad u \in \mathbf{U} \tag{12}$$

$$f_\mathrm{u}^\mathrm{WW} \leq n_\mathrm{u}^\mathrm{WW} \mathrm{WW}_\mathrm{u}^\mathrm{max} \quad u \in \mathbf{U} \tag{13}$$

where $F_\mathrm{u,u1}^\mathrm{max}$, $\mathrm{FW}_\mathrm{u}^\mathrm{max}$, and $\mathrm{WW}_\mathrm{u}^\mathrm{max}$ denote the upper bounds of $f_\mathrm{u,u1}$, $f_\mathrm{u}^\mathrm{FW}$, and $f_\mathrm{u}^\mathrm{WW}$, respectively. Obviously, the flow rate will be forced to zero if the corresponding binary variables are zero. Notice also that, in this study, the above-mentioned maximum flow rates are not just arbitrarily set to a sufficiently large value.[6] They are carefully chosen based on the design objective and also specifications of the water-using units. This practice is adopted to cut down search space and computation time. More details will be provided in the next section.

According to Yang et al.,[12] it is possible to obtain an optimal solution that contains a number of water streams with very low flow rates. To avoid this pitfall in network synthesis, the following constraints must also be introduced:

$$f_\mathrm{u,u1} \geq n_\mathrm{u,u1} F_{\mathrm{u,u}1}^\mathrm{min} \quad u,u1 \in \mathbf{U} \tag{14}$$

$$f_\mathrm{u}^\mathrm{FW} \geq n_\mathrm{u}^\mathrm{FW} \mathrm{FW}_\mathrm{u}^\mathrm{min} \quad u \in \mathbf{U} \tag{15}$$

$$f_\mathrm{u}^\mathrm{WW} \geq n_\mathrm{u}^\mathrm{WW} \mathrm{WW}_\mathrm{u}^\mathrm{min} \quad u \in \mathbf{U} \tag{16}$$

where $F_{\mathrm{u},u1}^\mathrm{min}$, $\mathrm{FW}_\mathrm{u}^\mathrm{min}$, and $\mathrm{WW}_\mathrm{u}^\mathrm{min}$ represent the lower bounds of $f_\mathrm{u,u1}$, $f_\mathrm{u}^\mathrm{FW}$, and $f_\mathrm{u}^\mathrm{WW}$, respectively.

Notice that the above formulation is essentially a MINLP problem. However, if the structural constraints are excluded, the remaining model forms a NLP.

## Initialization Strategy

Although the search space of the aforementioned NLP or MINLP problem is clearly defined, most solution procedures still call for a "good" initial guess. This is due to the fact that the starting point usually exerts a profound influence on the convergence process. Thus, a reliable initialization method has been developed in this work to satisfy this need.

Let us assume that the given data of the network synthesis problem include the following: the mass load of each contaminant in every water-using unit, the rate of water loss in each unit, and the upper bounds of the corresponding inlet and outlet concentrations. Based on these data, the following procedure can be followed to produce an initial guess:

**Step 1.** Determine the maximum freshwater consumption rate of each unit and assign it as the initial guess to $f_{\mathrm{u}}^{\mathrm{FW}}$.

Assume that wastewater reuse is not allowed and only one contaminant (say $k$) is considered, then the minimum freshwater consumption rate of unit $u$ can be determined if the maximum outlet concentration of contaminant $k$ is reached, i.e.,

$$G_{\mathrm{u,k}}^{\mathrm{FW}} = \frac{M_{\mathrm{u,k}}}{C\mathrm{out}_{\mathrm{u,k}}^{\max}} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{17}$$

here $C\mathrm{out}_{\mathrm{u,k}}^{\max}$ is the upper bound of outlet concentration, $G_{\mathrm{u,k}}^{\mathrm{FW}}$ is the minimum freshwater flow rate needed to satisfy the mass load of contaminant $k$ in unit $u$. For a water-using unit with multiple contaminants, the contaminant $k$ with maximum value of $G_{\mathrm{u,k}}^{\mathrm{FW}}$ is the key contaminant of unit $u$. Since the design objective is to minimize the total freshwater usage, the maximum freshwater consumption rate of unit $u$, denoted by $\mathrm{FW}_{\mathrm{u}}^{\max}$, should be

$$\mathrm{FW}_{\mathrm{u}}^{\max} = \max_{k} G_{\mathrm{u,k}}^{\mathrm{FW}} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{18}$$

Obviously, it is possible that there exist more than one key contaminant for a unit and the concentrations of the nonkey contaminants at the outlet do not reach their upper bounds when freshwater is supplied at the rate of $\mathrm{FW}_{\mathrm{u}}^{\max}$. So the initial value of $f_{\mathrm{u}}^{\mathrm{FW}}$ can be set to

$$(f_{\mathrm{u}}^{\mathrm{FW}}).l = \mathrm{FW}_{u}^{\max} \quad u \in \mathbf{U} \tag{19}$$

Here $(f_{\mathrm{u}}^{\mathrm{FW}}).l$ represents the initial value of $f_{\mathrm{u}}^{\mathrm{FW}}$ and the same notation is adopted throughout this paper.

**Step 2.** Set the initial guesses of $c_{\mathrm{u,k}}^{\mathrm{out}}$ and $f_{\mathrm{u,u1}}$. The necessary conditions of optimality[8] imply that the outlet concentration of at least one contaminant reaches its maximum. So the initial guess of $c_{\mathrm{u,k}}^{\mathrm{out}}$ is set to be $C\mathrm{out}_{\mathrm{u,k}}^{\max}$ temporally, i.e.,

$$(c_{\mathrm{u,k}}^{\mathrm{out}}).l = C\mathrm{out}_{\mathrm{u,k}}^{\max} \tag{20}$$

For an NLP or MINLP model, nonzero and reasonable initial values should be assigned to the flow rates of the interconnecting streams in the superstructure as much as possible. To maintain feasibility, the flow rate between any two units in the network should be set to zero on the basis of eq 19. However, it is desirable to provide a small nonzero flow rate for each $f_{\mathrm{u,u1}}$ to avoid zero derivatives. i.e.,

$$(f_{\mathrm{u,u1}}).l = \alpha \tag{21}$$

where $\alpha$ is a small adjustable positive parameter.

**Step 3.** Estimate the initial guesses of $f_{\mathrm{T}}^{\mathrm{FW}}$, $f_{\mathrm{u}}^{\mathrm{in}}$, $f_{\mathrm{u}}^{\mathrm{out}}$, $f_{\mathrm{u}}^{\mathrm{WW}}$, and $c_{\mathrm{u,k}}^{\mathrm{in}}$.

With the values of $(f_{\mathrm{u}}^{\mathrm{FW}}).l$, $(c_{\mathrm{u,k}}^{\mathrm{out}}).l$, and $(f_{\mathrm{u,u1}}).l$, the aforementioned variables can be initialized according to the following equality constraints:

$$(f_{\mathrm{T}}^{\mathrm{FW}}).l = \sum_{u=1}^{N_U} (f_{\mathrm{u}}^{\mathrm{FW}}).l \tag{22}$$

$$(f_{\mathrm{u}}^{\mathrm{in}}).l = \sum_{\substack{u1=1\\ u1\neq u}}^{N_{\mathrm{U}}} (f_{\mathrm{u1,u}}).l + (f_{\mathrm{u}}^{\mathrm{FW}}).l \quad u, u1 \in \mathbf{U} \tag{23}$$

$$(f_{\mathrm{u}}^{\mathrm{out}}).l = (f_{\mathrm{u}}^{\mathrm{in}}).l - F_{\mathrm{u}}^{\mathrm{L}} \quad u \in \mathbf{U} \tag{24}$$

$$(f_{\mathrm{u}}^{\mathrm{WW}}).l = (f_{\mathrm{u}}^{\mathrm{out}}).l - \sum_{\substack{u1=1\\ u1\neq u}}^{N_{\mathrm{u}}} (f_{\mathrm{u,u1}}).l \quad u, u1 \in \mathbf{U} \tag{25}$$

$$(c_{\mathrm{u,k}}^{\mathrm{in}}).l = \left(\sum_{\substack{u1=1\\ u1\neq u}}^{N_{\mathrm{U}}} (f_{\mathrm{u1,u}}).l(c_{\mathrm{u1,k}}^{\mathrm{out}}).l\right)/(f_{\mathrm{u}}^{\mathrm{in}}).l \quad u, u1 \in \mathbf{U}, k \in \mathbf{K} \tag{26}$$

**Step 4.** Modify the initial guess of $(c_{\mathrm{u,k}}^{\mathrm{out}}).l$. Usually, not all outlet concentrations reach their maximum; the value of every $(c_{\mathrm{u,k}}^{\mathrm{out}}).l$ can be corrected according to the following equation:

$$(c_{\mathrm{u,k}}^{\mathrm{out}}).l = ((f_{\mathrm{u}}^{\mathrm{in}}).l(c_{\mathrm{u,k}}^{\mathrm{in}}).l + M_{\mathrm{u,k}})/(f_{\mathrm{u}}^{\mathrm{out}}).l \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{27}$$

At this point, the initialization process for the NLP model is completed. For the MINLP model, the following steps should also be carried out:

**Step 5.** Initialize the binary variables.

$$(n_{\mathrm{u}}^{\mathrm{FW}}).l = 1 \quad (n_{\mathrm{u}}^{\mathrm{WW}}).l = 1 \quad u \in \mathbf{U} \tag{28}$$

$$(n_{\mathrm{u,u1}}).l = 1 \quad u, u1 \in \mathbf{U} \quad \text{and} \quad u \neq u1 \tag{29}$$

**Step 6.** Set the upper bounds of remaining flow rates, i.e., $F_{\mathrm{u,u1}}^{\max}$ and $\mathrm{WW}_{\mathrm{u}}^{\max}$.

Substitute eq 5 into eq 6 to eliminate the variable $f_{\mathrm{u}}^{\mathrm{in}}$ and then express $f_{\mathrm{u}}^{\mathrm{out}}$ as a function of the other variables, that is,

$$f_{\mathrm{u}}^{\mathrm{out}} = \frac{F_{\mathrm{u}}^{\mathrm{L}} c_{\mathrm{u,k}}^{\mathrm{in}} + M_{\mathrm{u,k}}}{c_{\mathrm{u,k}}^{\mathrm{out}} - c_{\mathrm{u,k}}^{\mathrm{in}}} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{30}$$

In this equation, if $c_{\mathrm{u,k}}^{\mathrm{out}}$ and $c_{\mathrm{u,k}}^{\mathrm{in}}$ simultaneously reach their maximum, the corresponding flow rate will be the limiting flow rate of unit $u$ when only contaminant $k$ is considered, i.e.,

$$F_{\mathrm{u,k}}^{\mathrm{lim}} = \frac{F_{\mathrm{u}}^{\mathrm{L}} C\mathrm{in}_{\mathrm{u,k}}^{\max} + M_{\mathrm{u,k}}}{C\mathrm{out}_{\mathrm{u,k}}^{\max} - C\mathrm{in}_{\mathrm{u,k}}^{\max}} \quad u \in \mathbf{U}, k \in \mathbf{K} \tag{31}$$

**Table 1. Stream Data of a Water-Using Network[2]**

| unit no. | unit | limiting flow rate (t/h) | contam | $Cin^{max}_{u,k}$ (ppm) | $Cout^{max}_{u,k}$ (ppm) |
|---|---|---|---|---|---|
| | | | hydrocarbon | 0 | 15 |
| 1 | distillation | 45 | $H_2S$ | 0 | 400 |
| | | | salt | 0 | 35 |
| | | | hydrocarbon | 20 | 120 |
| 2 | hydrodesul-furization | 34 | $H_2S$ | 300 | 12500 |
| | | | salt | 45 | 180 |
| | | | hydrocarbon | 120 | 220 |
| 3 | desalter | 56 | $H_2S$ | 20 | 45 |
| | | | Salt | 200 | 9500 |

**Table 2. Initial Guess Generated for Example 1**

| unit no. | $f_{u,u1}$ (t/h) | freshwater flow rate (t/h) | contam | $c^{in}_{u,k}$ (ppm) | $c^{out}_{u,k}$ (ppm) |
|---|---|---|---|---|---|
| | | | hydro-carbon | 0 | 15.00 |
| 1 | | 45.00 | $H_2S$ | 0 | 400.00 |
| | | | salt | 0 | 35.00 |
| | $F_{1,2} = 0.1$ | | hydro-carbon | 0.70 | 102.55 |
| 2 | $F_{3,2} = 0.1$ | 33.18 | $H_2S$ | 1.33 | 12426.45 |
| | | | salt | 28.56 | 166.05 |
| | $F_{1,3} = 0.1$ | | hydro-carbon | 0.25 | 102.03 |
| 3 | $F_{2,3} = 0.1$ | 54.82 | $H_2S$ | ***23.45*** | ***48.89*** |
| | | | salt | 0.39 | 9465.86 |
| total freshwater | 133.00 | | | | |

where $F^{lim}_{u,k}$ is the limiting flow rate of unit $u$ for contaminant $k$. The actual limiting flow rate of unit $u$ should be

$$Fout^{lim}_{u} = \max_{k \in K} F^{lim}_{u,k} \quad u \in \mathbf{U} \tag{32}$$

where $Fout^{lim}_{u}$ represents the limiting flow rate of unit $u$.

Since $F^{max}_{u,u1}$ and $WW^{max}_{u}$ represent the maximum flow rates of the branch streams connecting the splitting node of unit $u$ to the mixing nodes before unit $u1$ and wastewater sink respectively, they should equal to the corresponding limiting flowrate of unit $u$, i.e.,

$$F^{max}_{u,u1} = Fout^{lim}_{u} \quad WW^{max}_{u} = Fout^{lim}_{u} \quad u,u1 \in \mathbf{U} \tag{33}$$

## Illustrations

Two published examples are adopted here to illustrate the effectiveness of proposed initialization strategy. All models were solved by GAMS modules[14] (version 22.4) on an IBM notebook (model A22e).

**Example 1.** The WUN design problem presented here was originally studied by Wang and Smith[2] and later redesigned by Bagajewicz et al.[11] and Wang et al.[10] The given stream data are presented in Table 1. The design objective is to synthesize a network with minimum freshwater usage. The reported global optimum, which was identified with a tree-search method, calls for a consumption rate of 105.60 t/h.

The aforementioned NLP model (without the structure constraints) was formulated in the present example. The initial guesses were generated with the proposed method described in the previous section and the value of α was taken to be 0.1 t/h (see Table 2). It can be observed that these values are nearly feasible while the infeasible ones are given in boldfaced numbers. The module CONOPT3[14] was then used to solve the NLP problem. Notice also that, other than the freshwater stream, the flow rates of all input streams of unit 1 (i.e., distillation) were set to zero initially. This is due to the fact that the maximum allowable inlet concentrations of all contaminants in this unit should be zero and it is impossible to accept reused waters here.

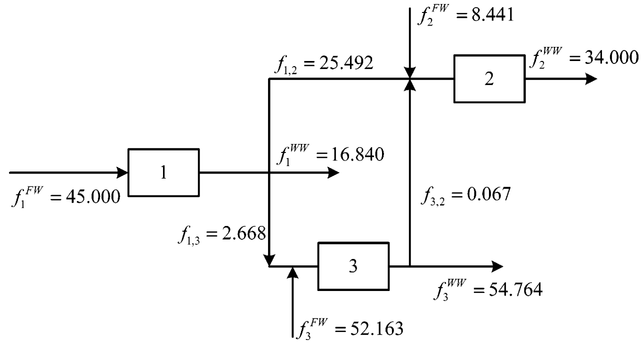


**Figure 2.** Optimum network for example 1.

**Table 3. Stream Data of Another Water-Using Network[11]**

| unit no. | contam | load (kg/h) | $Cin^{max}_{u,k}$ (ppm) | $Cout^{max}_{u,k}$ (ppm) |
|---|---|---|---|---|
| | A | 3.40 | 20 | 120 |
| 1 | B | 414.80 | 300 | 12500 |
| | C | 4.59 | 45 | 180 |
| | A | 5.60 | 120 | 220 |
| 2 | B | 1.40 | 20 | 1,000 |
| | C | 520.80 | 200 | 9500 |
| | A | 0.16 | 0 | 20 |
| 3 | B | 0.48 | 0 | 60 |
| | C | 0.16 | 0 | 20 |
| | A | 0.80 | 50 | 150 |
| 4 | B | 60.80 | 400 | 8000 |
| | C | 0.48 | 60 | 120 |
| | A | 0.75 | 0 | 15 |
| 5 | B | 20.00 | 0 | 400 |
| | C | 1.75 | 0 | 35 |
| | A | 2.00 | 10 | 70 |
| 6 | B | 100.70 | 200 | 600 |
| | C | 2.50 | 20 | 90 |
| | A | 1.80 | 25 | 150 |
| 7 | B | 6.80 | 230 | 1000 |
| | C | 0.60 | 20 | 220 |
| | A | 3.00 | 5 | 100 |
| 8 | B | 102.30 | 45 | 4000 |
| | C | 8.14 | 50 | 300 |
| | A | 4.60 | 13 | 100 |
| 9 | B | 200.00 | 200 | 3000 |
| | C | 1.90 | 5 | 200 |
| | A | 4.00 | 10 | 100 |
| 10 | B | 10.30 | 90 | 500 |
| | C | 9.00 | 70 | 800 |

**Table 4. Comparison the Optimum Network Obtained by Different Methods**

| method | objective value (t/h) | computing time (s) | no. of water reuse streams | min flow rate of reuse streams (t/h) |
|---|---|---|---|---|
| tree search[11] | 392.850 | <= 420 | 9 | 3.200 |
| NLP model | 390.849 | <=2 | 14 | 0.042 |
| MINLP model | 392.816 | <=4 | 10 | 1.000 |

The optimum network is found in 1 s with almost identical objective value, i.e., 105.604 t/h. This solution is presented in Figure 2. In addition, the same solution can also be found within 1 s with the other NLP solvers in GAMS, i.e., MINOS or SNOPT. Comparing with the tree search method[11] and the procedure-based method,[10] our proposed method is simpler and more efficient.

**Example 2.** A more complex water-using system is considered in this example. The stream data presented in Table 3 are

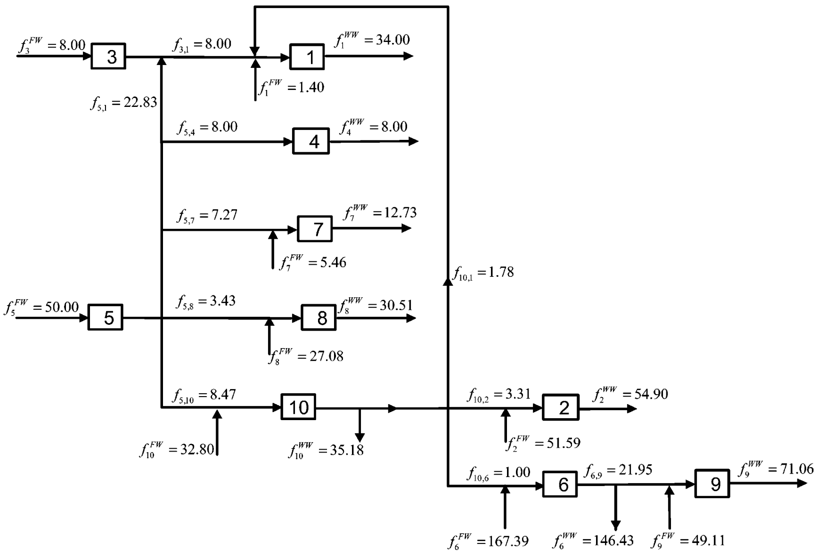


**Figure 3.** Optimum network obtained with MINLP model for example 2.

adopted from Bagajewicz et al.[11] The reported objective value is 392.85 t/h, and there are nine wastewater reuse streams in the corresponding network.

In our study, this WUN synthesis problem was solved with the proposed NLP and MINLP models separately to compare the effects of structural constraints. Since units 3 and 5 only accept pure waters, their input streams from other units in the superstructure were all removed. In addition, the structural constraints were not imposed upon the freshwater streams coming from the source and also wastewater streams discharging to the sink, that is, $n_u^{FW}$ and $n_u^{WW}$ do not appear on the left of eqs 9 and 10, respectively, and eqs 12, 13, 15, and 16 are not included in the MINLP model. This practice is due to the fact that, in a realistic chemical plant, the facilities to introduce freshwater and discharge wastewater are usually available for every water-using unit.

The NLP model was formulated without any structural constraint, and the value of $\alpha$ was chosen to be 2 t/h for generating the initial guesses. This model was then solved with MINOS, and the resulting minimum freshwater consumption rate was found to be 390.849 t/h. Notice that this result is slightly better than that reported in the literature. It should also be noted that the required computation time in the present case is much shorter (see Table 4). Finally, notice that additional suboptimal solutions can be found if $\alpha$ takes values other than 2 t/h; for example, the objective value is 394.779 t/h if $\alpha$ equals 1 t/h.

As for the MINLP-based synthesis approach, the value of $\alpha$ and the minimum flow rates of reuse streams, i.e., $F_{u,u1}^{min}$, were all set to be 1 t/h. The upper bounds $NM_u^{max}$ and $NS_u^{max}$ were all chosen to be 3 except that associated with the splitting node of unit 5; i.e., $NS_5^{max} = 5$. The reason for this choice is that the limiting throughput and also the maximum outlet concentrations of unit 5 are all quite moderate when compared with those of other units in the network, and thus, its wastewater has the highest potential to be reused. The NLP solver of MINOS and MIP solver of CPLEX are called in the MINLP solver of DICOPT. Under the aforementioned specifications, an optimal network can be identified. The key features of this solution can be found in Table 4. A more detailed version can be found in Figure 3 and Table 5. It can be observed from Table 4 that the number of reuse branches is reduced from 14 in the NLP solution to 10 in the MINLP solution, while the increase in the objective value in the latter case is ~0.5%. More importantly,

**Table 5. Optimum Network Obtained by MINLP Method for Example 2**

| process no. | $f_{u,u1}$ (t/h) | minimum freshwater flow rate (t/h) | contam | $c_{u,k}^{in}$ (ppm) | $c_{u,k}^{out}$ (ppm) |
|---|---|---|---|---|---|
| | $F_{3,1}$=8.000 | | A | 20.00 | 120.00 |
| 1 | $F_{5,1}$=22.828 | 1.396 | B | 300.00 | 12,500.00 |
| | $F_{10,1}$=1.776 | | C | 39.97 | 174.97 |
| | | | A | 6.03 | 108.04 |
| 2 | $F_{10,2}$=3.311 | 51.589 | B | 20.00 | 45.50 |
| | | | C | 13.59 | 9500.00 |
| | | | A | 0 | 20.00 |
| 3 | | 8.000 | B | 0 | 60.00 |
| | | | C | 0 | 20.00 |
| | | | A | 15.00 | 115.00 |
| 4 | $F_{5,4}$=8.000 | - | B | 400.00 | 8000.00 |
| | | | C | 35.00 | 95.00 |
| | | | A | 0 | 15.00 |
| 5 | | 50.000 | B | 0 | 400.00 |
| | | | C | 0 | 35.00 |
| | | | A | 0.60 | 12.47 |
| 6 | $F_{10,6}$=1.000 | 167.386 | B | 1.97 | 600.00 |
| | | | C | 1.34 | 16.19 |
| | | | A | 8.57 | 150.00 |
| 7 | $F_{5,7}$=7.273 | 5.455 | B | 228.57 | 762.86 |
| | | | C | 20.00 | 67.14 |
| | | | A | 1.69 | 100.00 |
| 8 | $F_{5,8}$=3.433 | 27.082 | B | 45.00 | 3397.46 |
| | | | C | 3.94 | 270.69 |
| | | | A | 3.85 | 68.59 |
| 9 | $F_{6,9}$=21.952 | 49.105 | B | 188.36 | 3000.00 |
| | | | C | 5.00 | 31.74 |
| | | | A | 3.08 | 100.00 |
| 10 | $F_{5,10}$=8.467 | 32.803 | B | 82.06 | 331.64 |
| | | | C | 7.18 | 225.26 |
| total freshwater | | 392.816 | | | |

notice the computation time for solving the more difficult MINLP model is still very short, i.e., less than 4 s.

## Conclusions

A simple and efficient initialization strategy is developed in this work to solve the NLP and MINLP models for synthesizing the optimal water-using networks with multiple contaminants. The NLP model is suitable for the relatively small-scale problems. Since the structural constraints are incorporated mainly for the purpose of simplifying network configuration, the MINLP model can be used to optimize larger water-using systems. Two examples from the literature are used to justify the proposed approach; the obtained optimum solutions are at least as good as the reported optimums but with significantly less computation time.

## Nomenclature

*Sets, Parameters, and Variables*

$\alpha$ = parameter used to initialize wastewater reuse stream
$N_K$ = the number of elements in set $K$
$N_U$ = the number of elements in set $U$
$c$ = concentration of contaminant
$C$in = given parameter of maximum concentration at inlet of a unit
$C$out = given parameter of maximum concentration at outlet of a unit
$f$ = flow rate of a water stream, t/h
$F$ = given parameter of flow rate parameter
FW = given parameter of flow rate of freshwater
$G$ = parameter of needed minimum flow rate of freshwater if no water reuse is allowed
$K$ = the set consists of contaminant
$M$ = parameter of mass load, kg/h
$n$ = binary variable to represent whether a water stream exists
NM = parameter to represent the number of branches entering a mixing node
NS = parameter to represent the number of branches leaving a splitting node
$U$ = the set consists of water-using units
WW = given parameter of flow rate of wastewater

*Superscripts*

FW = freshwater stream
in = inlet
L = loss
lim = limiting
max = maximum
min = minimum
out = outlet
WW = wastewater

*Subscripts*

k = the label of a contaminant
T = total amounts
u,u1 = the label of a water-using unit

## Acknowledgment

Financial support provided by Research Fund of Dalian Nationalities University under Grant 20056216 is gratefully acknowledged by the first author.

## Literature Cited

(1) Takama, T.; Kuriyama, T.; Shiroko. K.; Umeda. T. Optimal water allocation in a petroleum refinery. *Comput. Chem. Eng*. **1980**, *4*, 251.

(2) Wang, Y. P.; Smith, R. Wastewater minimization. *Chem. Eng. Sci.* **1994**, *49*, 981.

(3) Wang, Y. P.; Smith, R. Design of distributed effluent treatment systems. *Chem. Eng. Sci.* **1994**, *49*, 3127.

(4) Bagajewicz, M. A review of recent design procedures for water networks in refineries and process plants. *Comput. Chem. Eng.* ***2000****, 24* (9), 2093.

(5) Li, B. H.; Fei, W. Y. Design water-using network with multiple contaminants by step by step linear programming. *J. Chem. Ind. Eng.* **2005**, *56* (2), 285. (In Chinese).

(6) Zheng, X. S.; Feng, X.; Shen, R. J.; Seider, W. D. Design of optimal water-using networks with internal water mains. *Ind. Eng. Chem. Res.* **2006**, *45* (25), 8413.

(7) Savelski, M. J.; Bagajewicz, M. J. On the optimality conditions of water utilization systems in process plants with single contaminants. *Chem. Eng. Sci.* **2000**, *55*, 5035.

(8) Savelski, M. J.; Bagajewicz, M. J. On the necessary conditions of optimality of water utilization systems in process plants with multiple contaminants. *Chem. Eng. Sci.* **2003**, *58*, 5349.

(9) Savelski, M. J.; Bagajewicz, M. J. Algorithmic procedure to design water utilization systems featuring a single contaminant in process plants. *Chem. Eng. Sci.* **2001**, *56*, 1897.

(10) Wang, B.; Feng, X.; Zhang, Z. X. A design methodology for multiple-contaminant water networks with single internal water main. *Comput. Chem. Eng.* **2003**, *27*, 903.

(11) Bagajewicz, M. J.; Rivas, M.; Savelski, M. J. A new approach to the design of water utilization systems with multiple contaminants in process plants. Annual AIChE Meeting 1999, Dallas, TX, 1999.

(12) Yang, Y. H.; Lou, H. H.; Huang, Y. L. Synthesis of an optimal wastewater reuse network. *Waste Manage.* **2000**, *20*, 311.

(13) Chang, C. T.; Li, B. H. Improved optimization strategies for generating practical water-usage and -treatment network structures. *Ind. Eng. Chem. Res*. **2005**, *44*, 3607.

(14) GAMS Development Corp. GAMS: The solver manuals. GAMS Development Corp.: Washington DC, 2005.

*Received for review* May 16, 2007
*Revised manuscript received* September 2, 2007
*Accepted* September 11, 2007

IE070702Y