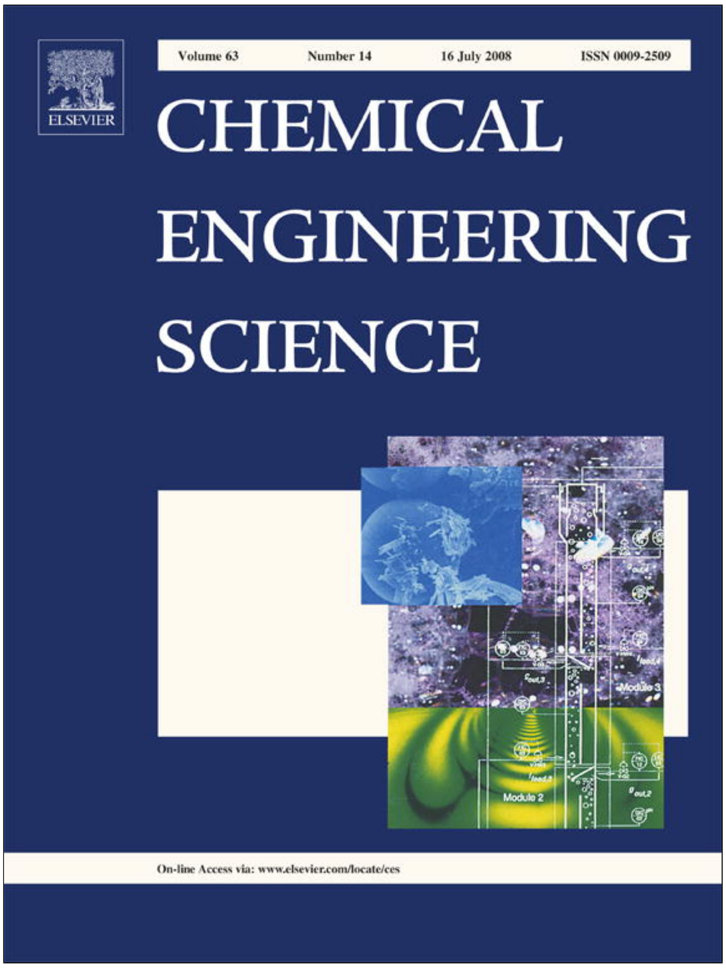
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Simultaneous optimization approach for integrated water-allocation and heat-exchange networks

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ABSTRACT

A systematic design methodology is developed in this work for simultaneously synthesizing the multi-contaminant water-allocation and heat exchange network (WAHEN) in any chemical process. Specifically, a modified state-space representation is adopted to capture the structural characteristics of the integrated WAHEN, and a mixed-integer nonlinear program (MINLP) is formulated accordingly to minimize the total annualized cost (TAC) of the network design. In the proposed mathematical programming model, not only all possible water reuse and treatment options are incorporated, but also the direct and indirect heat-exchange opportunities are considered as well. To enhance the solution quality and efficiency, a stochastic perturbation procedure is introduced to generate reliable initial guesses for the deterministic optimization procedures and also, an interactive iteration method is developed to guide the search toward a potential global optimum. Three examples are presented in this paper to demonstrate the validity and advantages of the proposed approach.

1. Introduction

Water and energy are two of the most essential resources for running chemical processing plants. The former is needed not only as a solvent in mass-transfer processes but also as a heat-transfer medium in heat exchangers. Specifically, various organic and inorganic contaminants in another phase can often be removed with process water. Thus, clean water is widely considered as an effective mass-separating agent in washing or separation operations (such as absorption and extraction). In addition, the aerated and purified water is consumed in the utility systems to produce steam and/or cooling water for use as heat carriers. After the aforementioned usages, the resulting wastewaters must be treated to lower the contaminant concentrations. Some of them can then be recycled and reused, while the others discharged to the environment. Bagajewicz (2000) presented a comprehensive review of the available design procedures for water networks and the potential research opportunities on heat integration.

Although the water and energy management issues in every chemical process are always highly related, the design problems of water-allocation networks (WANs) and heat-exchange networks (HENs) have been considered separately in the past (Takama et al., 1980; Linnhoff and Hindmarsh, 1983; Yee and Grossmann, 1990; Wang and Smith, 1994a, b; Alva-Argaez et al., 1998; Huang et al., 1999; Karuppiah and Grossman, 2006). The former networks were synthesized with nonlinear programming (NLP) models, while the latter were designed with mixed integer nonlinear programs (MINLP). However, since the water-using units and wastewater-treatment units are often required to be operated at different temperatures, a strong interaction does exist between the corresponding WAN and HEN designs.

Savulescu and Smith (1998) and Savulescu et al. (2005a, b) proposed a conceptual design method, i.e., the water-energy pinch analysis, to solve the combined WAN–HEN optimization problem The so-called *separate system approach* was adopted to create the overall network design with a graphic tool—the two-dimensional grid diagram. Although both direct and indirect heat-exchange options have been considered in their work (Savulescu et al., 2002), it is still very difficult to incorporate all possible network configurations and to identify an optimal solution with the minimum total annualized cost (TAC) using this heuristic approach. On the other hand, Bagajewicz et al. (2002) tried to solve the same problem with mathematical programming models. They developed a series of transshipment formulations on the basis of the optimality conditions for water-using networks (Savelski and Bagajewicz, 2000). In these models, the process-to-process connection streams were allowed to be heated/cooled with heat exchangers. However, since the original

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nonlinear functions in NLP and MINLP models were linearized, the true optimal design may not be identifiable by using this method. Notice also that the aforementioned two approaches are really not applicable to the multi-contaminant problems that is usually encountered in the process industries and, more importantly, both are in essence sequential procedures. Their common main drawback is that the trade-offs between capital investments and operating costs, i.e., those associated with freshwater and heating and cooling utilities, cannot be properly balanced. To circumvent this problem, Du et al. (2004) studied a multi-contaminant WAN–HEN design problem by repeatedly solving MINLP models via adaptive simulated annealing and genetic algorithms (GA/SA). Although a simultaneous optimization strategy was adopted in this work, the required computation load was extremely heavy and the direct heat-exchange opportunities were ignored completely. Finally, it should be noted that none of the above studies include wastewater-treatment systems in the WAN–HEN designs There is therefore a need to develop a more comprehensive design method for optimizing the integrated water-allocation and heat-exchange networks (WAHENs).

To illustrate the WAHEN design method developed in this work, the rest of this paper is organized as follows. The WAHEN design problem is formally defined in the next section. As mentioned previously in abstract, the state-space concept (Bagajewicz and Manousiouthakis, 1992; Bagajewicz et al., 1998) is adopted and modified in the present study to construct a superstructure for capturing the unique characteristics of generalized WAHEN configuration. This modified state-space representation and the corresponding MINLP model are described in Section 3. A hybrid optimization strategy has also been developed to solve the proposed model and an outline of the solution algorithm can be found in the following section. Three examples are then presented in Section 5 to demonstrate the feasibility and effectiveness of the proposed solution method. The capabilities of the state-space based model can also be clearly observed from the resulting network designs Finally the conclusions of this research and some comments on future works are provided in the last section.

2. Problem statement

The water-using units and wastewater-treatment units in a chemical plant are usually selected on the basis of process requirements and also government regulations on effluents. The operating temperatures of these units are dictated by the need to optimize process performance. Thus, it may be necessary to heat/cool the water streams in a WAHEN due to the temperature differences between two adjacent units, between a source and a unit, and between a unit and a sink. To facilitate a concise formulation of the mathematical model, the following simplification assumptions are introduced in this study:

- The WAHEN process is continuous.
- Each unit is operated isothermally without water loss and heat loss.
- Only the water streams and the heating and cooling utilities are considered in HEN design. Other hot and cold process streams are excluded for the sake of simplicity

A general WAHEN design problem can be stated as follows: Given a set of freshwater sources, a set of wastewater sinks, a set of hot and cold utilities, a set of existing water-using units and a set of available wastewater-treatment units, it is desired to synthesize a cost-optimal WAHEN that can fulfill the mass-load requirements of all water-using units and also satisfy the concentration, temperature and flow-rate constraints imposed at various locations in the network.

The given model parameters of this optimization problem include: (1) the design specifications of every water-using unit (i.e., its operating temperature, its mass-loads for all contaminants, and the corresponding upper concentration bounds at inlet and/or outlet), (2) the design specifications of every wastewater-treatment unit (i.e., its operating temperature, its throughput limit, the removal ratios of all contaminants, and the corresponding upper concentration bounds at inlet and/or outlet), (3) the temperature and contaminant concentrations at every source and its highest supply rate, (4) the maximum allowable temperature, discharge rate and contaminant concentrations at every sink, (5) the temperature levels of the hot and cold utilities and (6) the heat capacities of all water streams and the estimates of overall heat-transfer coefficients in all heat exchangers.

The resulting WAHEN design should include: (1) the throughput of every water-using unit, (2) the number of wastewater-treatment units and their throughputs, (3) the number of heat exchangers and their duties, (4) the consumption rates of freshwaters, and the hot and cold utilities, (5) the discharge rates of wastewaters and their temperatures and contaminant concentrations at the sinks, and (6) the complete network configuration and the flow rate of each branch stream.

3. Model formulation

The state-space superstructure was proposed by Bagajewicz and Manousiouthakis (1992) and Bagajewicz et al. (1998) as an alternative representation of the mass exchange network and HEN. Bagajewicz et al. (2002) applied this concept to integrate a water-using network with a HEN in order to minimize the freshwater and energy consumption rates of the combined system. This original structure has been improved in the present work to incorporate additional design options, e.g., the distributed wastewater-treatment and direct heat-exchange operations. More specifically, the WAHEN is viewed as a system of two interconnected blocks (see Fig. 1). One is referred to as the distribution network (DN), in which all mixers, splitters and the connections between them are embedded. The other is the so-called process operator (OP), which can be further divided into two sub-blocks, i.e., OP-WAN and OP-HEN. All water users and potential wastewater-treatment units are placed in the former sub-block, while all *indirect* heat-exchange opportunities are provided in the latter. Their inner stream connections and the corresponding mathematical models are described in the sequel.

3.1. Distribution network

Only the freshwater streams and the cold and hot utility streams can be considered as the *external* inputs to DN block, while the recycle streams from the OP block are treated as the *internal* inputs. Every input is split into several branches and each of them is connected to a mixer at the exit leading to one of the OP sub-blocks or to the environment. These splitters and mixers are divided into three groups depending upon their original identities or their connections with the units in the OP block. In the following equations the subscript w is used to represent a water source or sink while w' and w'' are used to represent water streams connected to the water-using or wastewater-treatment units in OP_WAN; subscript i denotes a hot utility stream, while i' and i'' are the labels of hot process streams connected to the heat exchangers in OP_HEN; subscript j denotes a cold utility stream, while j' and j'' are the labels of cold process streams connected to the heat exchangers in OP_HEN. Notice that, at every splitter and mixer, the water contaminant and energy balances must all be satisfied, i.e.,

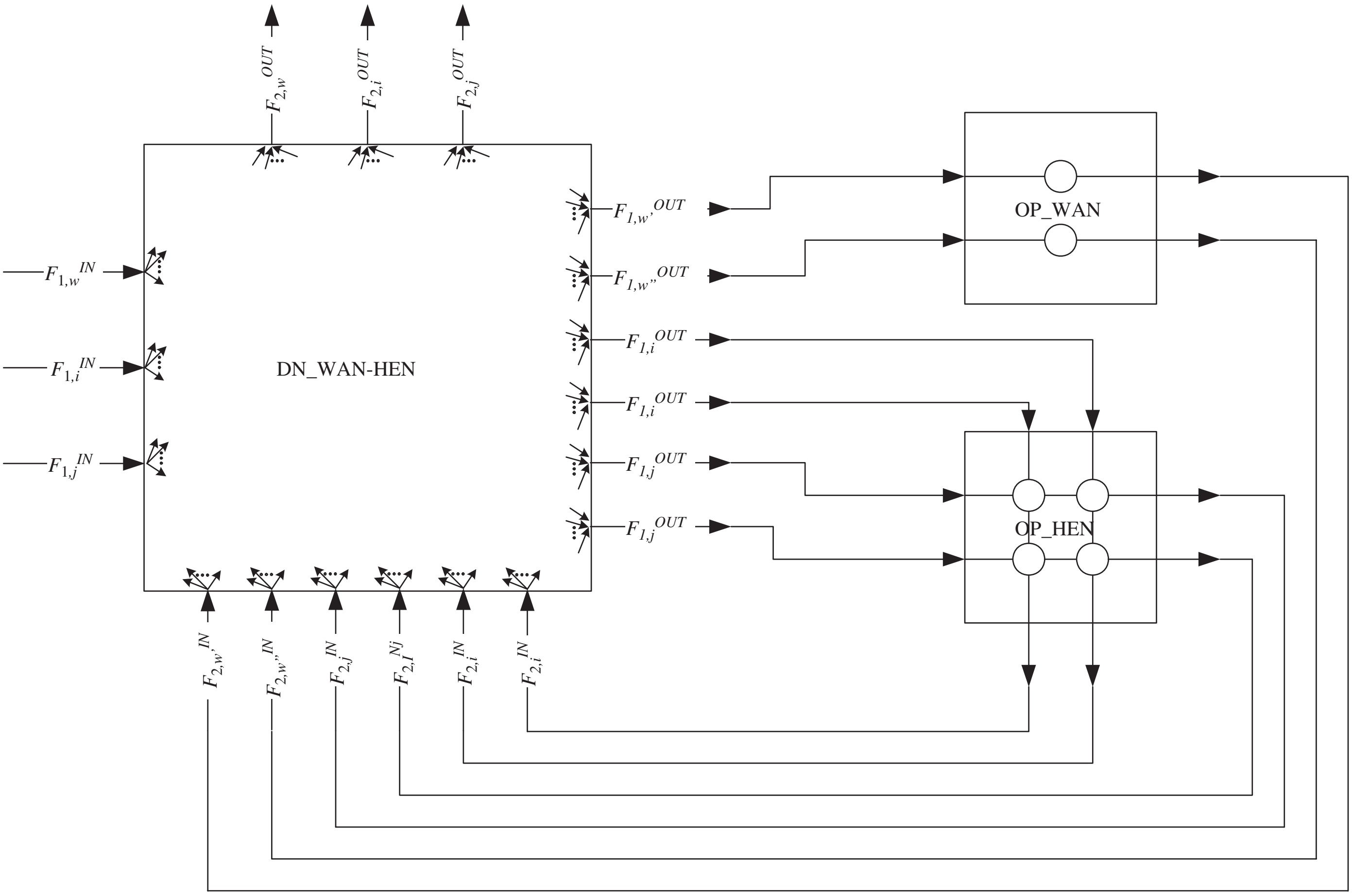

Fig. 1. State-space representation of WAHEN.

$$F_{1,w}^{\mathrm{IN}} = \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{1,w,l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{1,w,k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{1,w,g} + \sum_{h=1}^{W_2^{\mathrm{out}}} f_{1,w,h}, \quad w = 1, 2, \ldots, W_1^{\mathrm{in}} \tag{1}$$

$$F_{1,i}^{\mathrm{IN}} = \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{1,i,l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{1,i,k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{1,i,g} + \sum_{h=1}^{W_2^{\mathrm{out}}} f_{1,i,h}, \quad i = 1, 2, \ldots, M_1^{\mathrm{in}} \tag{2}$$

$$F_{1,j}^{\mathrm{IN}} = \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{1,j,l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{1,j,k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{1,j,g} + \sum_{h=1}^{W_2^{\mathrm{out}}} f_{1,j,h}, \quad j = 1, 2, \ldots, N_1^{\mathrm{in}} \tag{3}$$

$$F_{1,w'}^{\mathrm{OUT}} = \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w'} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w'} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w'} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w'} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w'} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w'}, \quad w' = 1, 2, \ldots, W_1^{\mathrm{out}} \tag{4}$$

$$F_{1,w'}^{\mathrm{OUT}} T_{1,w'}^{\mathrm{OUT}} = \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w'} T_{1,k}^{\mathrm{IN}} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w'} T_{1,l}^{\mathrm{IN}} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w'} T_{2,k}^{\mathrm{IN}} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w'} T_{2,l}^{\mathrm{IN}} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w'} T_{1,g}^{\mathrm{IN}} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w'} T_{2,h}^{\mathrm{IN}}, \quad w' = 1, 2, \ldots, W_1^{\mathrm{out}} \tag{5}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,w'}C^{\mathrm{OUT}}_{1,w',s} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w'}C^{\mathrm{IN}}_{1,k,s} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w'}C^{\mathrm{IN}}_{1,l,s}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w'}C^{\mathrm{IN}}_{2,k,s} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w'}C^{\mathrm{IN}}_{2,l,s}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w'}C^{\mathrm{IN}}_{1,g,s} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w'}C^{\mathrm{IN}}_{2,h,s},\\ & s=1,2,\ldots,S,\quad w'=1,2,\ldots,W_1^{\mathrm{out}}\end{aligned}\tag{6}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,i'} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i'} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i'} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i'}\\ &+ \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i'} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i'} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i'},\\ & i'=1,2,\ldots,M_1^{\mathrm{out}}\end{aligned}\tag{7}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,i'}T^{\mathrm{OUT}}_{1,i'} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i'}T^{\mathrm{IN}}_{1,k} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i'}T^{\mathrm{IN}}_{1,l}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i'}T^{\mathrm{IN}}_{2,k} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i'}T^{\mathrm{IN}}_{2,l}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i'}T^{\mathrm{IN}}_{1,g} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i'}T^{\mathrm{IN}}_{2,h},\\ & i'=1,2,\ldots,M_1^{\mathrm{out}}\end{aligned}\tag{8}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,i'}C^{\mathrm{OUT}}_{1,i',s} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i'}C^{\mathrm{IN}}_{1,k,s} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i'}C^{\mathrm{IN}}_{1,l,s}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i'}C^{\mathrm{IN}}_{2,k,s} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i'}C^{\mathrm{IN}}_{2,l,s}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i'}C^{\mathrm{IN}}_{1,g,s} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i'}C^{\mathrm{IN}}_{2,h,s},\\ & s=1,2,\ldots,S,\quad i'=1,2,\ldots,M_1^{\mathrm{out}}\end{aligned}\tag{9}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,j'} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j'} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j'} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j'}\\ &+ \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j'} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j'} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j'},\\ & j'=1,2,\ldots,N_1^{\mathrm{out}}\end{aligned}\tag{10}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,j'}T^{\mathrm{OUT}}_{1,j'} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j'}T^{\mathrm{IN}}_{1,k} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j'}T^{\mathrm{IN}}_{1,l}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j'}T^{\mathrm{IN}}_{2,k} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j'}T^{\mathrm{IN}}_{2,l}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j'}T^{\mathrm{IN}}_{1,g} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j'}T^{\mathrm{IN}}_{2,h},\\ & j'=1,2,\ldots,N_1^{\mathrm{out}}\end{aligned}\tag{11}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{1,j'}C^{\mathrm{OUT}}_{1,j',s} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j'}C^{\mathrm{IN}}_{1,k,s} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j'}C^{\mathrm{IN}}_{1,l,s}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j'}C^{\mathrm{IN}}_{2,k,s} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j'}C^{\mathrm{IN}}_{2,l,s}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j'}C^{\mathrm{IN}}_{1,g,s} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j'}C^{\mathrm{IN}}_{2,h,s},\\ & s=1,2,\ldots,S,\quad j'=1,2,\ldots,N_1^{\mathrm{out}}\end{aligned}\tag{12}$$

$$\begin{aligned}F^{\mathrm{IN}}_{2,w'} ={}& \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{2,w',l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{2,w',k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{2,w',g}\\ &+ \sum_{h=1}^{W_2^{\mathrm{out}}} f_{2,w',h},\quad w'=1,2,\ldots,W_2^{\mathrm{in}}\end{aligned}\tag{13}$$

$$\begin{aligned}F^{\mathrm{IN}}_{2,i'} ={}& \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{2,i',l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{2,i',k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{2,i',g}\\ &+ \sum_{h=1}^{W_2^{\mathrm{out}}} f_{2,i',h},\quad i'=1,2,\ldots,M_2^{\mathrm{in}}\end{aligned}\tag{14}$$

$$\begin{aligned}F^{\mathrm{IN}}_{2,j'} ={}& \sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} f_{2,j',l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} f_{2,j',k} + \sum_{g=1}^{W_1^{\mathrm{out}}} f_{2,j',g}\\ &+ \sum_{h=1}^{W_2^{\mathrm{out}}} f_{2,j',h},\quad j'=1,2,\ldots,N_2^{\mathrm{in}}\end{aligned}\tag{15}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{2,w} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w}\\ &+ \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w},\\ & w=1,2,\ldots,W_2^{\mathrm{out}}\end{aligned}\tag{16}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{2,w}T^{\mathrm{OUT}}_{2,w} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w}T^{\mathrm{IN}}_{1,k} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w}T^{\mathrm{IN}}_{1,l}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w}T^{\mathrm{IN}}_{2,k} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w}T^{\mathrm{IN}}_{2,l}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w}T^{\mathrm{IN}}_{1,g} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w}T^{\mathrm{IN}}_{2,h},\\ & w=1,2,\ldots,W_2^{\mathrm{out}}\end{aligned}\tag{17}$$

$$\begin{aligned}F^{\mathrm{OUT}}_{2,w}C^{\mathrm{OUT}}_{2,w,s} ={}& \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,w}C^{\mathrm{IN}}_{1,k,s} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,w}C^{\mathrm{IN}}_{1,l,s}\\ &+ \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,w}C^{\mathrm{IN}}_{2,k,s} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,w}C^{\mathrm{IN}}_{2,l,s}\\ &+ \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,w}C^{\mathrm{IN}}_{1,g,s} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,w}C^{\mathrm{IN}}_{2,h,s},\\ & s=1,2,\ldots,S,\quad w=1,2,\ldots,W_2^{\mathrm{out}}\end{aligned}\tag{18}$$

$$\begin{aligned} F_{2,i}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i} \\ & + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i}, \\ & i = 1, 2, \ldots, M_2^{\mathrm{out}} \end{aligned} \tag{19}$$

$$\begin{aligned} F_{2,i}^{\mathrm{OUT}} T_{2,i}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i} T_{1,k}^{\mathrm{IN}} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i} T_{1,l}^{\mathrm{IN}} \\ & + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i} T_{2,k}^{\mathrm{IN}} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i} T_{2,l}^{\mathrm{IN}} \\ & + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i} T_{1,g}^{\mathrm{IN}} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i} T_{2,h}^{\mathrm{IN}}, \\ & i = 1, 2, \ldots, M_2^{\mathrm{out}} \end{aligned} \tag{20}$$

$$\begin{aligned} F_{2,i}^{\mathrm{OUT}} C_{2,i,s}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,i} C_{1,k,s}^{\mathrm{IN}} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,i} C_{1,l,s}^{\mathrm{IN}} \\ & + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,i} C_{2,k,s}^{\mathrm{IN}} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,i} C_{2,l,s}^{\mathrm{IN}} \\ & + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,i} C_{1,g,s}^{\mathrm{IN}} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,i} C_{2,h,s}^{\mathrm{IN}}, \\ & s = 1, 2, \ldots, S, \quad i = 1, 2, \ldots, M_2^{\mathrm{out}} \end{aligned} \tag{21}$$

$$\begin{aligned} F_{2,j}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j} + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j} \\ & + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j} + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j}, \\ & j = 1, 2, \ldots, N_2^{\mathrm{out}} \end{aligned} \tag{22}$$

$$\begin{aligned} F_{2,j}^{\mathrm{OUT}} T_{2,j}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j} T_{1,k}^{\mathrm{IN}} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j} T_{1,l}^{\mathrm{IN}} \\ & + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j} T_{2,k}^{\mathrm{IN}} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j} T_{2,l}^{\mathrm{IN}} \\ & + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j} T_{1,g}^{\mathrm{IN}} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j} T_{2,h}^{\mathrm{IN}}, \\ & j = 1, 2, \ldots, N_2^{\mathrm{out}} \end{aligned} \tag{23}$$

$$\begin{aligned} F_{2,j}^{\mathrm{OUT}} C_{2,j,s}^{\mathrm{OUT}} = {} & \sum_{k=1}^{M_1^{\mathrm{in}}} f_{1,k,j} C_{1,k,s}^{\mathrm{IN}} + \sum_{l=1}^{N_1^{\mathrm{in}}} f_{1,l,j} C_{1,l,s}^{\mathrm{IN}} \\ & + \sum_{k=1}^{M_2^{\mathrm{in}}} f_{2,k,j} C_{2,k,s}^{\mathrm{IN}} + \sum_{l=1}^{N_2^{\mathrm{in}}} f_{2,l,j} C_{2,l,s}^{\mathrm{IN}} \\ & + \sum_{g=1}^{W_1^{\mathrm{in}}} f_{1,g,j} C_{1,g,s}^{\mathrm{IN}} + \sum_{h=1}^{W_2^{\mathrm{in}}} f_{2,h,j} C_{2,h,s}^{\mathrm{IN}}, \\ & s = 1, 2, \ldots, S, \quad j = 1, 2, \ldots, N_2^{\mathrm{out}} \end{aligned} \tag{24}$$

where $F_{p,w}^{\mathrm{IN}}$, $F_{p,i}^{\mathrm{IN}}$ and $F_{p,j}^{\mathrm{IN}} (p = 1, 2)$ represent, respectively, the mass flow rates of the wth water stream, the ith hot stream and the jth cold stream entering DN for the pth time; $F_{p,w}^{\mathrm{OUT}}$, $F_{p,i}^{\mathrm{OUT}}$ and $F_{p,j}^{\mathrm{OUT}} (p = 1, 2)$ denote, respectively, the mass flow rates of the wth water stream, the ith hot stream and the jth cold stream leaving DN for the pth time; $f_{p,q,r}$ $(p = 1, 2)$ is the flow rate of a branch from the qth splitter to the rth mixer; W_p^{IN}, M_p^{IN} and $N_p^{\mathrm{IN}} (p = 1, 2)$ represent the numbers of inlet splitters for the water, hot and cold streams, respectively, entering the DN for the pth time; W_p^{OUT}, M_p^{OUT} and N_p^{OUT} $(p = 1, 2)$, respectively, represent the numbers of outlet mixers of the water, hot and cold streams. Notice that, for a given design problem, the numbers of exterior junctions to and from environment are fixed, i.e.,$W_1^{\mathrm{IN}} = W_2^{\mathrm{OUT}} = W_{\mathrm{ext}}$, $M_1^{\mathrm{IN}} = M_2^{\mathrm{OUT}} = M_{\mathrm{ext}}$ and $N_1^{\mathrm{IN}} = N_2^{\mathrm{OUT}} = N_{\mathrm{ext}}$ are constants. On the other hand, the numbers of interior junctions to and from the OP block are *adjustable* parameters, i.e.,$W_1^{\mathrm{out}} = W_2^{\mathrm{in}} = W_{\mathrm{int}}$, $M_1^{\mathrm{out}} = M_2^{\mathrm{in}} = M_{\mathrm{int}}$ and $N_{1,j}^{\mathrm{out}} = N_{2,j}^{\mathrm{in}} = N_{\mathrm{int}}$ should be chosen by the designer(s). Consequently,

$$F_{1,w}^{\mathrm{OUT}} = F_{2,w}^{\mathrm{IN}} = F_w \tag{25}$$

$$F_{1,i}^{\mathrm{OUT}} = F_{2,i}^{\mathrm{IN}} = F_i \tag{26}$$

$$F_{1,j}^{\mathrm{OUT}} = F_{2,j}^{\mathrm{IN}} = F_j \tag{27}$$

Finally, there are of course additional constraints imposed at the sources, i.e.,

$$F_{1,q}^{\mathrm{IN}} \leqslant F_q^{\mathrm{source}} \quad (q = w, i \text{ or } j) \tag{28}$$

$$T_{1,q}^{\mathrm{IN}} = T_q^{\mathrm{source}} \quad (q = w, i \text{ or } j) \tag{29}$$

$$C_{1,w,s}^{\mathrm{IN}} = C_{w,s}^{\mathrm{source}} \tag{30}$$

where F_q^{source}denotes the upper flow limits of the supply rate at source q, T_q^{source} is the temperature at source q, $C_{w,s}^{\mathrm{source}}$ is the concentration of contaminant s at source w. A set of similar constraints can also be imposed at the sinks, i.e.,

$$F_{2,w}^{\mathrm{OUT}} \leqslant F_w^{\mathrm{sink}} \tag{31}$$

$$T_{2,w}^{\mathrm{OUT}} \leqslant T_w^{\mathrm{sink}} \tag{32}$$

$$T_{2,q'}^{\mathrm{OUT}} = T_{q'}^{\mathrm{sink}} \quad (q' = i \text{ or } j) \tag{33}$$

$$C_{2,w,s}^{\mathrm{OUT}} \leqslant C_{w,s}^{\mathrm{sink}} \tag{34}$$

where F_w^{sink}, T_w^{sink} and $C_{w,s}^{\mathrm{sink}}$, respectively, represent the upper bounds of the flow rate, temperature and concentration of contaminant s at the wastewater sink w and $T_{q'}^{\mathrm{sink}}$ denotes the temperature of heating or cooling utility at sink q'.

3.2. Process operator

The energy balance round each exchanger in OP_HEN can be written as

$$F_i Cp_i (T_i^{\mathrm{in}} - T_i^{\mathrm{out}}) - F_j Cp_j (T_j^{\mathrm{out}} - T_j^{\mathrm{in}}) = 0, \quad i \in \Gamma_H, \ j \in \Gamma_C \tag{35}$$

where Γ_H and Γ_C denote, respectively, the sets of process streams coming from the hot-stream and cold-stream mixers of DN block, F_i and F_j denote the flow rates of hot and cold streams, respectively and Cp_i and Cp_j are the corresponding specific heats. The heat-transfer area needed for each match can be calculated according to the following equation:

$$F_j Cp_j (T_j^{\text{out}} - T_j^{\text{in}}) - U_{i,j} A_{i,j} \Delta \underset{i,j}{\bar{T}} = 0, \quad i \in \Gamma_H,\ j \in \Gamma_C \tag{36}$$

where $U_{i,j}$ is the overall heat-transfer coefficient, $A_{i,j}$ the heat-transfer area and $\Delta\bar{T}_{i,j}$ the log-mean temperature difference in the exchanger. Finally, notice that the above two equations are valid only when the corresponding match is active. This requirement can be described by introducing binary variables into the inequality constraints established according to the second law of thermodynamics, i.e.,

$$T_j^{\text{in}} - T_i^{\text{out}} \leqslant M_{i,j}(1 - z_{i,j}), \quad i \in \Gamma_H,\ j \in \Gamma_C \tag{37}$$

$$T_j^{\text{out}} - T_i^{\text{in}} \leqslant M'_{i,j}(1 - z_{i,j}), \quad i \in \Gamma_H,\ j \in \Gamma_C \tag{38}$$

$$T_i^{\text{out}} - T_i^{\text{in}} \leqslant 0, \quad i \in \Gamma_H \tag{39}$$

$$T_j^{\text{in}} - T_j^{\text{out}} \leqslant 0, \quad i \in \Gamma_C \tag{40}$$

where $z_{i,j}$ is a binary variable reflecting whether or not the match between streams i and j exists and $M_{i,j}$ and $M'_{i,j}$ are two large enough positive constants. Notice that, in this model, every hot stream is allowed to be matched with more than one cold stream and vice versa. This practice is adopted to improve the search efficiency in solution process (Papalexaddri and Pistikopoulos, 1994; Dong et al., 2008).

The water-using operations in OP_WAN are assumed to be always present. The mass balance for every water-using unit can thus be formulated without using a binary variable, i.e.,

$$F_u (C_{u,s}^{\text{out}} - C_{u,s}^{\text{in}}) = \Delta m_{u,s}, \quad u \in \Gamma_U,\ s \in \Omega \tag{41}$$

where Γ_U represents the set of process streams coming from the exit mixers which are dedicated to the water-using operations, Ω is the set of all contaminants and $C_{u,s}^{\text{in}}$ and $C_{u,s}^{\text{out}}$ denote, respectively, the concentrations of contaminant s at the inlet and outlet of water user on stream u. On the other hand, since not all available wastewater-treatment units are required to be selected in the final design, the corresponding model formulation should be

$$\begin{aligned} &C_{t,s}^{\text{in}} - C_{t,s}^{\text{out}} - \varphi_{t,s} Y_{t,s} = 0 \\ &(y_t - 1)U_t \leqslant Y_{t,s} - C_{t,s}^{\text{in}} \leqslant (1 - y_t)U_t \\ &0 \leqslant Y_{t,s} \leqslant y_t Y_t^{\max} \\ &s \in \Omega, \quad t \in \Gamma_t \end{aligned} \tag{42}$$

where Γ_T represents the set of process streams coming from the exit mixers which are dedicated to the wastewater-treatment operations, y_t is the binary variable reflecting whether or not the treatment unit on stream t exists, $\varphi_{t,s}$ is the removal ratio of contaminant s in the treatment unit on stream t, $C_{t,s}^{\text{in}}$ and $C_{t,s}^{\text{out}}$ denote the corresponding concentrations at the inlet and outlet of treatment unit and $Y_{t,s}$ is an artificial variable which equals $C_{t,s}^{\text{in}}$ only when $y_t = 1$; $Y_t^{\max}$ is an arbitrarily selected large constant. Finally, the additional constraints on temperatures and concentrations in OP_WAN can be written as

$$C_{w,s}^{\text{in}} \leqslant \bar{C}_{w,s}^{\text{in}}, \quad C_{w,s}^{\text{out}} \leqslant \bar{C}_{w,s}^{\text{out}}, \quad w \in \Gamma_U \cup \Gamma_T,\ s \in \Omega \tag{43}$$

$$T_w^{\text{in}} = T_w^{\text{out}} = \bar{T}_w, \quad w \in \Gamma_U \cup \Gamma_T,\ s \in \Omega \tag{44}$$

where $\bar{C}_{w,s}^{\text{in}}$, $\bar{C}_{w,s}^{\text{out}}$ and $\bar{T}_w$are given constants.

3.3. Connection junctions

As mentioned previously, the numbers of interior junctions, i.e.,W_{int}, M_{int} and N_{int}, must be chosen to facilitate satisfactory solution of the state-space model. To address this issue, let us consider these numbers individually. Generally speaking, the presence of every water-using unit is dictated by process requirements. Thus, the number of junctions connected to the water-using units can be obviously fixed first so as to ensure a one-to-one correspondence between them. On the other hand, the water-treatment units used in the state-space model can be viewed as off-line equipments available for possible installation. As long as the environmental regulations are satisfied, the number of repeated units may be less than that in the superstructure and it may not even be necessary to use every type of unit in the optimum solution. The appropriate number of repeated units for each type of treatment operation in the OP block can be determined with the heuristic rules proposed by Chang and Li (2005). For illustration convenience, the total number of available treatment units is denoted as size (Γ_T). Thus,

$$W_{\text{int}} = \text{size}(\Gamma_U) + \text{size}(\Gamma_T) \tag{45}$$

where size(Γ_U) represents the total number of existing water-using units.

On the other hand, it is also imperative to place additional interior junctions to provide enough opportunities to match the hot and cold streams in the sub-block OP_HEN. Since the numbers of hot and cold streams in WAHEN cannot be determined in advance, the corresponding junction numbers can only be estimated heuristically by enumeration. In this study, it has been found that these numbers should be chosen within the following ranges:

$$\text{size}^2(\Gamma_U) \leqslant M_{\text{int}} \leqslant [\text{size}(\Gamma_U) + \text{size}(\Gamma_T)]^2 \tag{46}$$

$$\text{size}^2(\Gamma_U) \leqslant N_{\text{int}} \leqslant [\text{size}(\Gamma_U) + \text{size}(\Gamma_T)]^2 \tag{47}$$

The upper and lower bounds here can be obtained by counting all possible connections between water-using and/or wastewater-treatment units. The optimal WAHEN can be identified by the selecting the numbers of interior junctions for hot and cold streams and then solving the corresponding MINLP model in a trial-and-error fashion. The values of M_{int} and N_{int} should be increased one-at-a-time from their lower limits.

4. Interactive solution strategy

Engineering optimization problems are often formulated as non-convex MINLPs. Recent developments on the stochastic and deterministic algorithms for solving MINLP models have been thoroughly reviewed by Pardalos et al. (2000) and Floudas et al. (2005). It is well recognized that none of the available generic methods can be applied successfully to all chemical process synthesis problems without the aid of case-specific insights. The proposed WAHEN optimization algorithm includes three distinct components. The first is designed to produce feasible solutions with randomly generated initial guesses; the second is used to improve the candidate solution(s) with perturbation techniques; the third is aimed to produce alternative network structures (mainly HEN) evolutionarily by shifting heat loads in loops and along utility paths. The detailed solution steps are given in the flowchart shown in Fig. 2. The DICOPT solver (Viswanathan and Grossmann, 1990) in GAMS is used in this procedure to solve the MINLP models and it is interfaced with MATLAB (Ferris, 2005) for executing various initiation and perturbation steps in the first and second components. Also, to improve the preliminary HEN structure in the integrated WAHEN, heat loads are shifted around loops and along paths to reduce exchanger number (Su and Motard, 1984) in the third component. Aspen's Engineering Suite is adopted in this work to implement the needed evolutionary procedure. Notice that, although the solution steps within each component can be performed automatically, the above optimization strategy still has to be executed interactively between different components at locations A, B,

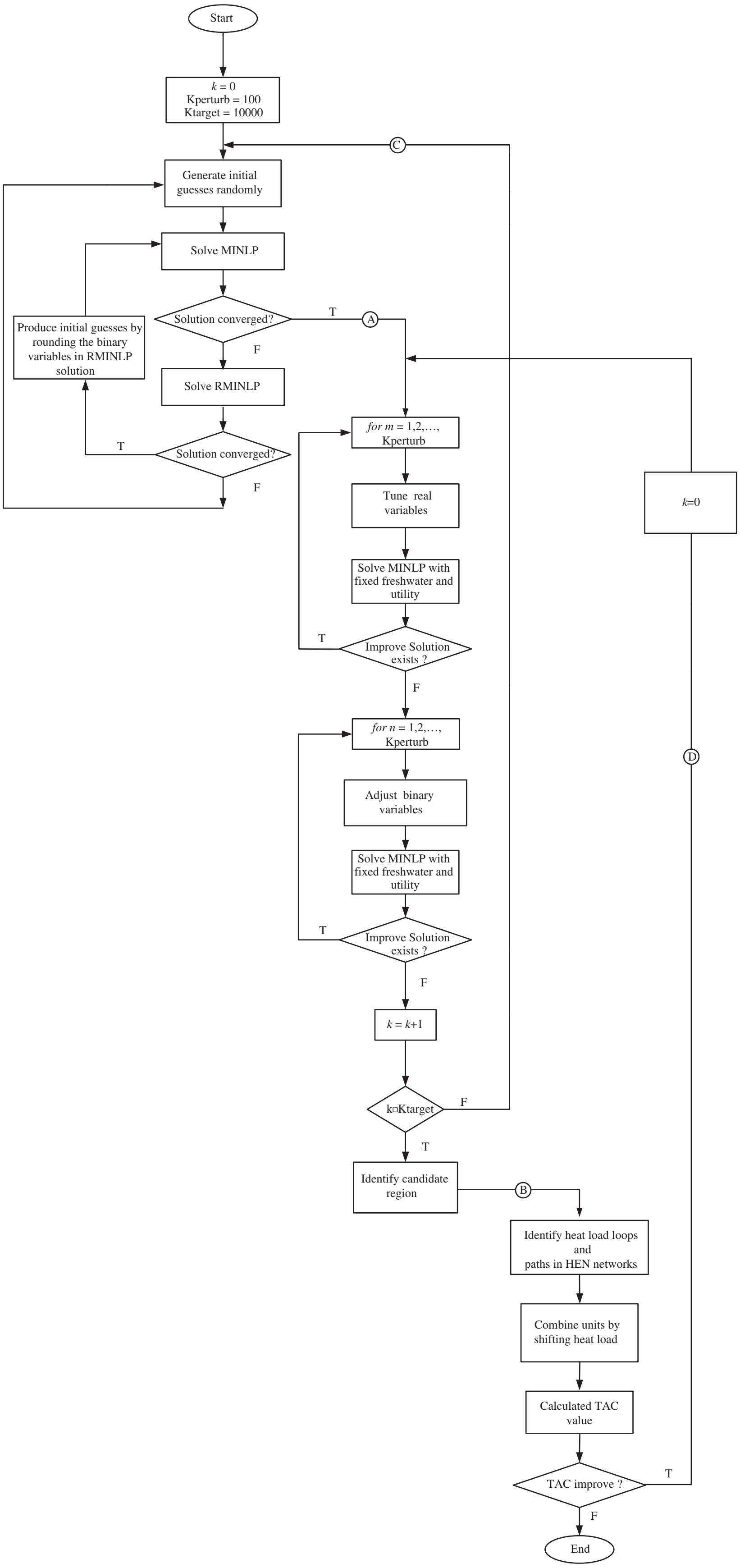

Fig. 2. Interactive solution strategy.

C and D so as to monitor the solution performance and to judicially interfere and/or control the solution process.

Before carrying out the proposed solution procedure, it is helpful to first determine the upper and lower bounds of freshwater and utility consumption rates. In this work, these bounds are calculated sequentially. In particular, an optimal WAN is first synthesized by solving a NLP model (Huang et al., 1999) to minimize the freshwater supply rate. The resulting objective value is used as the lower bound. On the other hand, the maximum flow rate of freshwater can be determined by excluding all wastewater-treatment units and all water-reuse opportunities. On the basis of the assumptions that only freshwater is consumed in every water user and also one of the outlet concentrations reaches the upper limit, the upper bound of freshwater consumption rate can be computed by summing the water flow rates in all water-using units. Having fixed the WAN configurations, the stream data of the subsequent HEN design problem can then be identified accordingly. In this work, the upper bounds of utility consumption rates are calculated by excluding all heat-exchange opportunities in HEN. On the other hand, the minimum utility consumption rates are computed by allowing zero minimum temperature approach in mixers with a LP model (Chang and Chen, 1997)

The first step in component 1 of the proposed procedure is to produce a set of initial guesses of the decision variables with a random number generator. In the MINLP model, these decision variables are chosen to be the binary variables, i.e., z_{ij}s and y_ts and also the split ratios of all splitters. The latter are real variables defined as

$$\varphi_{p,q,r} = \frac{f_{p,q,r}}{F^{\mathrm{IN}}_{p,q}} \tag{48}$$

where $\varphi_{p,q,r}$ denotes the split ratio of a branch leaving the splitter on the qth water/hot/cold stream entering from environment ($p=1$) and from OP block ($p=2$), respectively to, the rth outlet mixer. Notice that Eqs. (1)–(3) and (13)–(15) can be re-written in a unified format according to the following definition:

$$\sum_{l=1}^{M_1^{\mathrm{out}}+N_1^{\mathrm{out}}} \varphi_{p,q,l} + \sum_{k=1}^{M_2^{\mathrm{out}}+N_2^{\mathrm{out}}} \varphi_{p,q,k} + \sum_{g=1}^{W_1^{\mathrm{out}}} \varphi_{p,q,g} + \sum_{h=1}^{W_2^{\mathrm{out}}} \varphi_{p,q,h} = 1 \tag{49}$$

where $p = 1, 2$ and $q = 1, 2, \ldots, W_p^{\mathrm{in}}$ (or M_p^{in}, or N_p^{in}). The primary objective at this point is to obtain the feasible solution of the original MINLP problem directly with the randomly generated initial guesses. If this is not possible, a relaxed MINLP is then solved with the same initial guesses. If this attempt is successful, the solution of this RMINLP is then slightly modified to create an additional set of initial guesses for the original MINLP problem. In particular, if a relaxed binary variable is found to be close to 1 (say, larger than 0.7), the corresponding initial value can be set to one. A similar practice can be used to set the initial value of a close-to-zero (say, less than 0.3) binary variable. The remaining relaxed binary variables should be left unspecified. However, if the solution process of the RMINLP model is not convergent, the search procedure in component 1 should be restarted by generating another set of initial guesses randomly.

It is well established that the numerical iteration process in solving a MINLP problem is highly dependent upon the initial guesses and may converge to a local optimum. To enhance the solution quality, new initial guesses are thus created in the second component by introducing random perturbations into the initial feasible solutions. In addition, the original MINLP model is also modified by fixing the freshwater and utility levels at those in the selected initial solution. This modified model is then solved with the perturbed initial guesses to search for improved solutions. More specifically, the initial split ratios are adjusted according to the following equation:

$$\varphi_{p,q,r} = \varphi^{I}_{p,q,r}(1 + \varepsilon_{p,q,r}) \tag{50}$$

where $\varphi^{I}_{p,q,r}$ denotes the split ratio in the component-1 solution and $\varepsilon_{p,q,r}$ is a randomly generated perturbation in the interval $[-\delta, +\delta]$ and usually $\delta = 0.05$. On the other hand, the binary variables are adjusted one-at-a-time. Each time one of the binary variables is selected randomly. Its value is then changed from 0 to 1 or vice versa.

As mentioned previously, the HEN structure is improved in the third component by breaking heat load loops. Since this evolutionary technique is well known, a detailed description of the implementation steps is omitted for the sake of brevity. With the help of case-specific insights, the solution process can be made more efficient by driving the search to a much more restricted region, which cannot otherwise be discovered with an automatic computer algorithm.

5. Application example

Following examples are presented to illustrate the capabilities of the modified state-space model and the effectiveness of the proposed solution strategy. Example 1 was originally solved with a sequential procedure based on the pinch analysis by Savulescu and Smith (1998) and Savulescu et al. (2005a, b), or with the mathematical programming models by Bagajewicz et al. (2002). Example 2 was studied by Bagajewicz et al. (2002) without considering the wastewatertreatment options. Example 3 is a multi-contaminant water network design problem adopted from Mann and Liu (1999). This system was later integrated with HEN by Du et al. (2004), but the direct heatexchange opportunities were ignored completely.

A set of common model parameters are used in all three examples. Specifically, the unit prices for the primary and secondary waters are chosen to be 0.375 and 0.45 USD ton^{-1}, respectively; the inlet and outlet temperatures of cooling water are set at 10 and 20 °C, respectively, and its cost is 189 USD kW^{-1} yr^{-1}; the temperatures of low and medium-pressure steams are assumed to be 120 and 150 °C, respectively, and the corresponding costs are 377 and 388 USD kW^{-1} yr^{-1}; the overall heat-transfer coefficient is assumed to be 0.5 kW/m^2 °C; the annualized capital-cost model for a conventional shell-and-tube heat exchanger is $8000z_{i,j} + 1200A_{i,j}^{0.6}$ where the heat-transfer area $A_{i,j}$ is in m^2 (Ahmad et al., 1990; Linnhoff and Ahmad, 1990). Finally, the annual interest rate is set at 10% and the plant is assumed to be operated continuously for 8000 h a year.

5.1. Example 1

Let us first consider the process data presented in Table 1 (Savulescu and Smith, 1998; Bagajewicz et al., 2002; Savulescu et al., 2005a, b). As mentioned before, the wastewater-treatment operations were not considered in this problem. To be able to compare different strategies on the same basis, let us assume that TACs of the published network structures can be calculated according to the aforementioned cost models. Based on the conceptual design method, Savulescu et al. (2005a, b) obtained a WAHEN design which

Table 1
Process data of Example 1

Unit (u)	Δm_u (g s^{-1})	$\bar{C}_u^{\mathrm{in}}$ (mg l^{-1})	$\bar{C}_u^{\mathrm{out}}$ (mg l^{-1})	f_u^{lim} (kg s^{-1})	$\bar{T}_u$ (°C)
1	2	0	100	20	40
2	5	50	100	100	100
3	30	50	800	40	75
4	4	400	800	10	50

Temperature of primary water = 20 °C; maximum wastewater temperature = 30 °C.

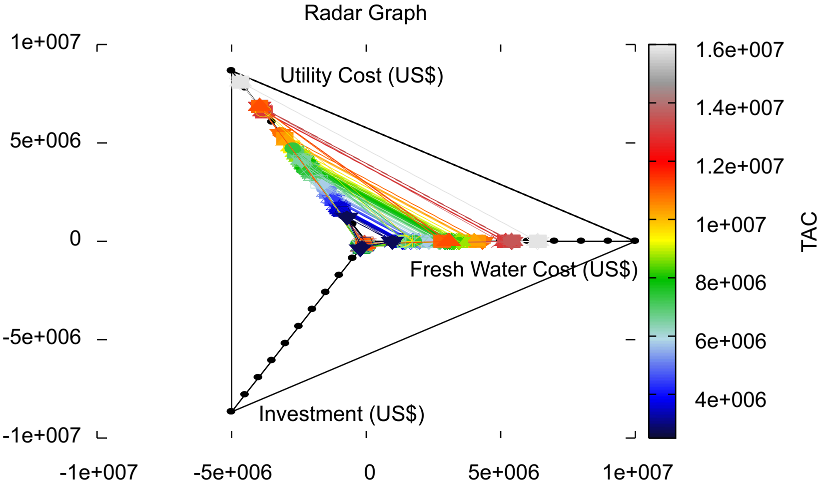

Fig. 3. Radar graph showing distributions of TAC, freshwater cost, utility cost and capital investment.

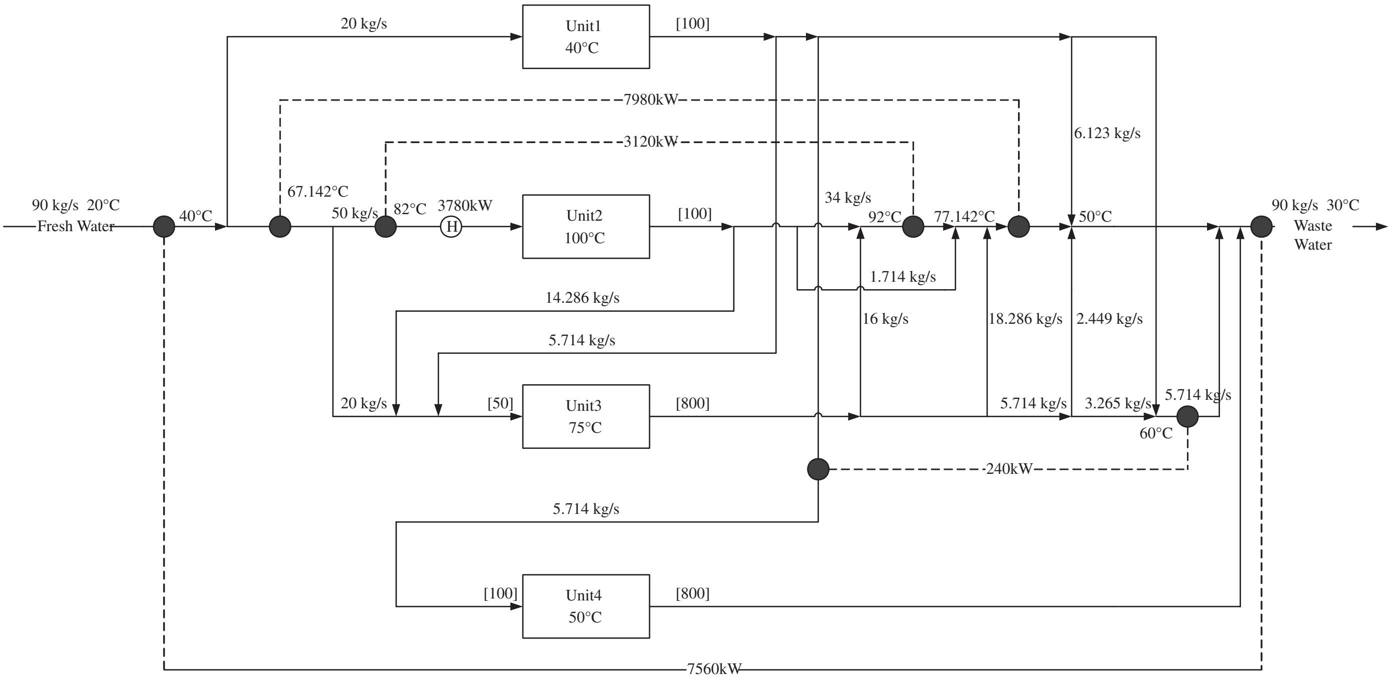

Fig. 4. An optimal WAHEN design in Example 1.

consumes the smallest amount of freshwater (90 kg s^{-1}). There is 1 cooler and 1 heater in this network, but no exchangers are needed. The TAC and the annualized capital investment of this system are estimated to be 2,769,314 and 50829 USD yr^{-1}, respectively. The corresponding consumption rates of cooling water and hot utility (MP steam) are 485 and 4265 kW, respectively On the other hand, with the mathematical programming models, Bagajewicz et al. (2002) synthesized another WAHEN which requires the same freshwater supply rate. Three heat exchangers and one heater are needed in this design. The estimated TAC and annualized capital investment in this case are 2,711,555 and 314495 USD yr^{-1}, respectively. The corresponding consumption rate of hot utility (LP steam) is 3780 kW.

A total of 441 different optimal WAHEN designs have also been generated for this example on the basis of the proposed state-space model. The distribution of their TACs, as well as the corresponding freshwater cost, utility cost and capital investment, can be visualized through a radar graph (see Fig. 3). It can be observed that the freshwater and utility expenditures are the main contributors of TAC, while the capital investment plays a relatively minor role. Notice also that the smallest TAC obtained with the proposed approach is approximately the same as those mentioned above. One of the networks is presented in Fig. 4, in which four heat exchangers and one heater are used. The TAC and the annualized capital investment in this case were found to be 2738107.4 and 341, 047.4 USD yr^{-1}, respectively. Notice that the corresponding consumption rates of the hot utility (LP steam) and freshwater, i.e., 3780 kW and 90 kg s^{-1} are the same as those estimated for the design reported in Bagajewicz et al. (2002).

Although the minimum TACs achieved with different approaches are roughly the same in the present example, it is still more advantageous to follow the modeling and solution strategies proposed in this work. This is due to the fact that multiple design alternatives can be conveniently generated for practical applications. Furthermore, the simultaneous optimization strategy adopted in the present study is believed to be more effective in handling the trade-off between the capital and operating costs. This assertion can also be verified later in the following example.

5.2. Example 2

Let us next consider the process data presented in Table 2 (Bagajewicz et al., 2002). In the original case study, only the freshwater consumption rate was calculated and its value is 77.3 kg s^{-1}. Notice also that the wastewater-treatment options were not considered and no concentration limits were imposed upon the sink.

In Case I of the present example, the sequential solution procedure suggested by Bagajewicz et al. (2002) is followed to integrate the water-using network with a HEN. More specifically, a NLP model is solved first to synthesize a water network with minimize freshwater usage and then a MINLP model is solved accordingly to obtain a HEN with minimum utility cost. The resulting network structure is shown in Fig. 5, in which four heat exchangers, one cooler and two heaters are included. Its TAC and the corresponding capital investment were found to be 2,742,198.4 and 406, 290.8 USD yr^{-1}, respectively. The freshwater flow rate in this design is 77.3 kg s^{-1}, while the consumption rates of cold and hot utilities (LP steam) are 491 and 3736.2 kW, respectively.

Table 2
Process data of Example 2

Unit (u)	Δm_u (g s^{-1})	$\bar{C}_u^{\mathrm{in}}$ (mg l^{-1})	$\bar{C}_u^{\mathrm{out}}$ (mg l^{-1})	f_u^{lim} (kg s^{-1})	$\bar{T}_u$ (°C)
1	5	50	100	100	100
2	30	50	800	40	75
3	50	800	1100	166.7	100

Temperature of primary water = 20 °C; maximum wastewater temperature = 30 °C.

The same WAHEN design problem is solved in Case II with simultaneous solution strategy. Specifically, a single state-space MINLP is solved to obtain the design with minimum TAC. The resulting network structure is presented in Fig. 6, in which two heat exchangers and two heaters are used. Its TAC and the corresponding capital investment were found to be 2,631,805.4 and 305, 913.3 USD yr^{-1}, respectively. The freshwater flow rate in this design is 87.2 kg s^{-1}, while the consumption rate of hot utility (LP steam) is 3,671.4 kW.

A comparison of the key features of the above two designs is summarized in Table 3. It can be concluded that the simultaneous optimization strategy is clearly superior to a sequential one. This is due to the fact that the trade-off issues in WAHEN design can be better addressed with the former approach. Specifically, although the consumption rate of freshwater in Case I is less than that in Case II, the utility consumption level and the capital investment in the former case are both drastically reduced so as to lower TAC significantly in the latter case.

To demonstrate the capability of state-space superstructure for incorporating the wastewater-treatment options in WAHEN design, an additional case study (Case III) is performed by imposing an extra upper bound of 20 ppm on the contaminant concentration at the sink. In addition, it is assumed that two classes of wastewater-treatment processes are available for the present system, their removal ratios are 95% and 90%, respectively, and their operating temperatures are both required to be maintained at 30 °C. The cost models of these treatment units are adopted from Kuo and Smith (1998). The capital costs (USD yr^{-1}) are determined according to the formulas $16800F_t^{0.7}$ and $12600F_t^{0.7}$, while the corresponding operating costs (USD yr^{-1}) are calculated with the formulas F_t and $0.76F_t$, respectively. In these formulas, the symbol F_t represents the throughput of treatment unit t in ton h^{-1}. The state-space superstructure for this case is shown in Fig. 7. Notice that, although all splitters and

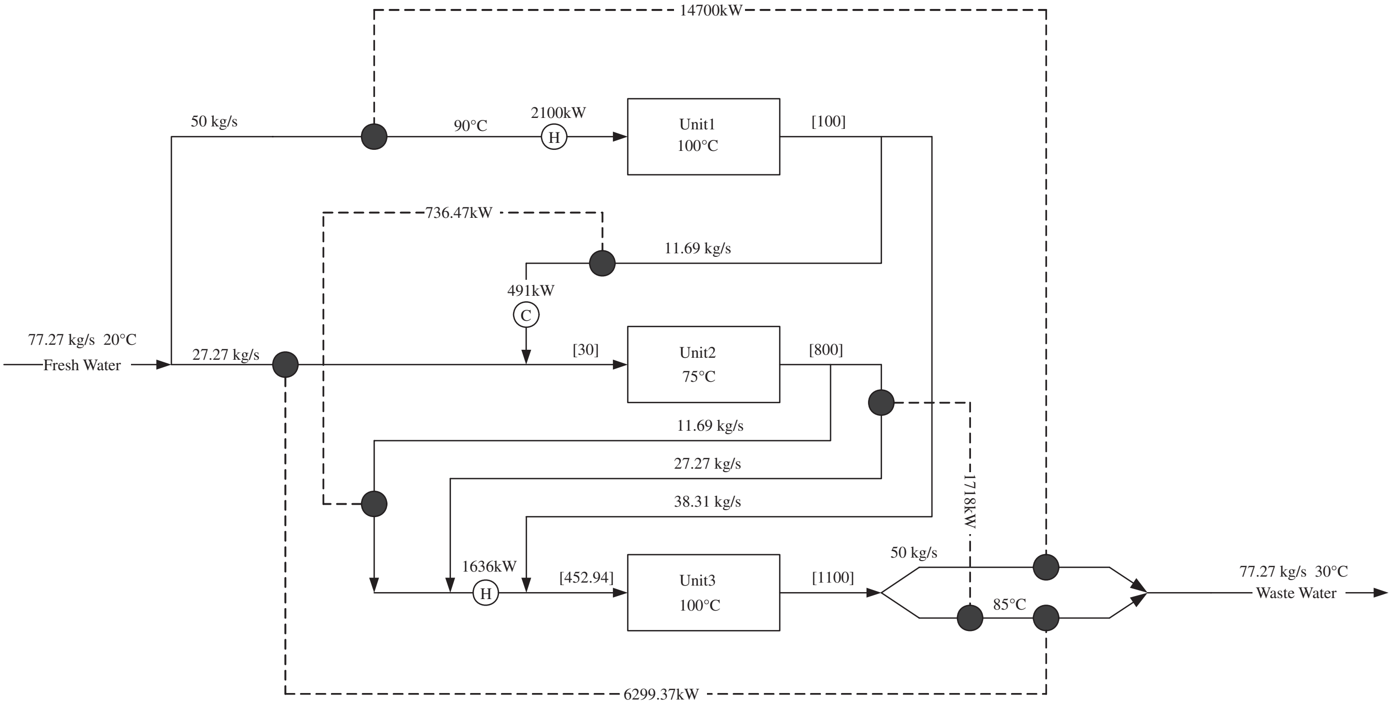

Fig. 5. Optimal WAHEN design for Case I in Example 2.

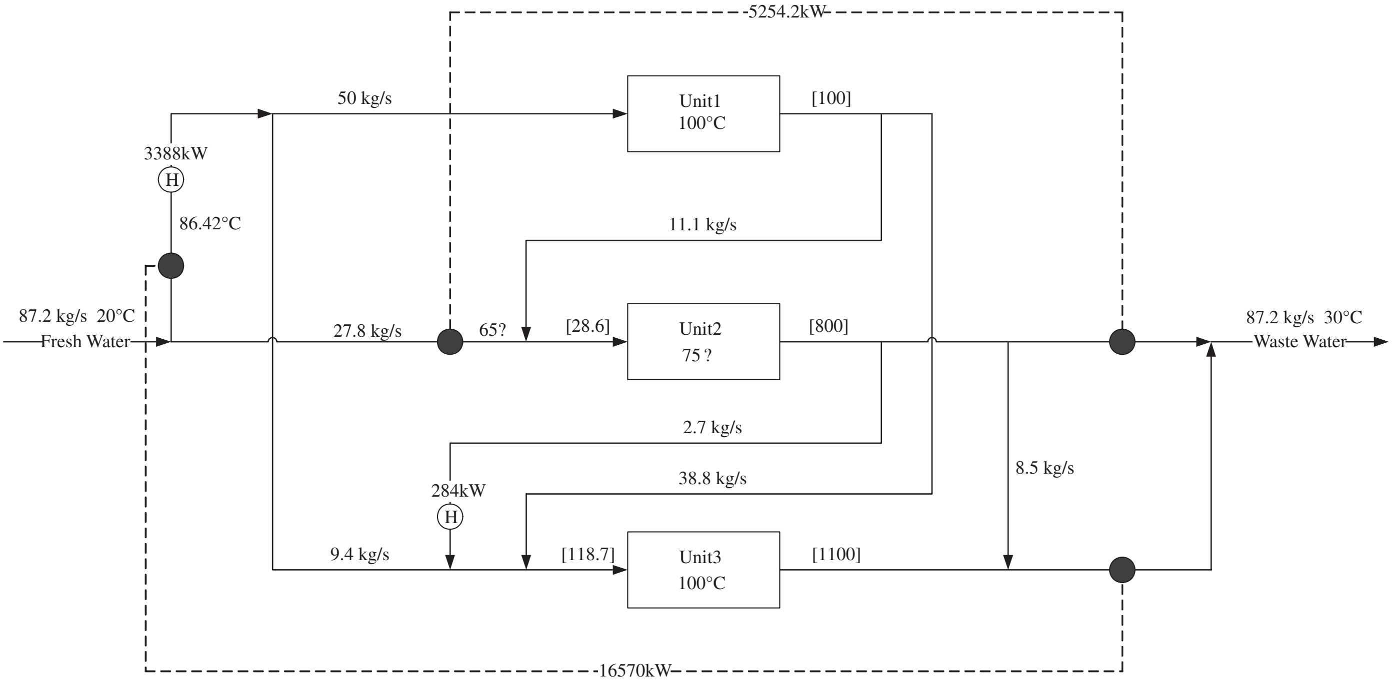

Fig. 6. Optimal WAHEN design for Case II in Example 2.

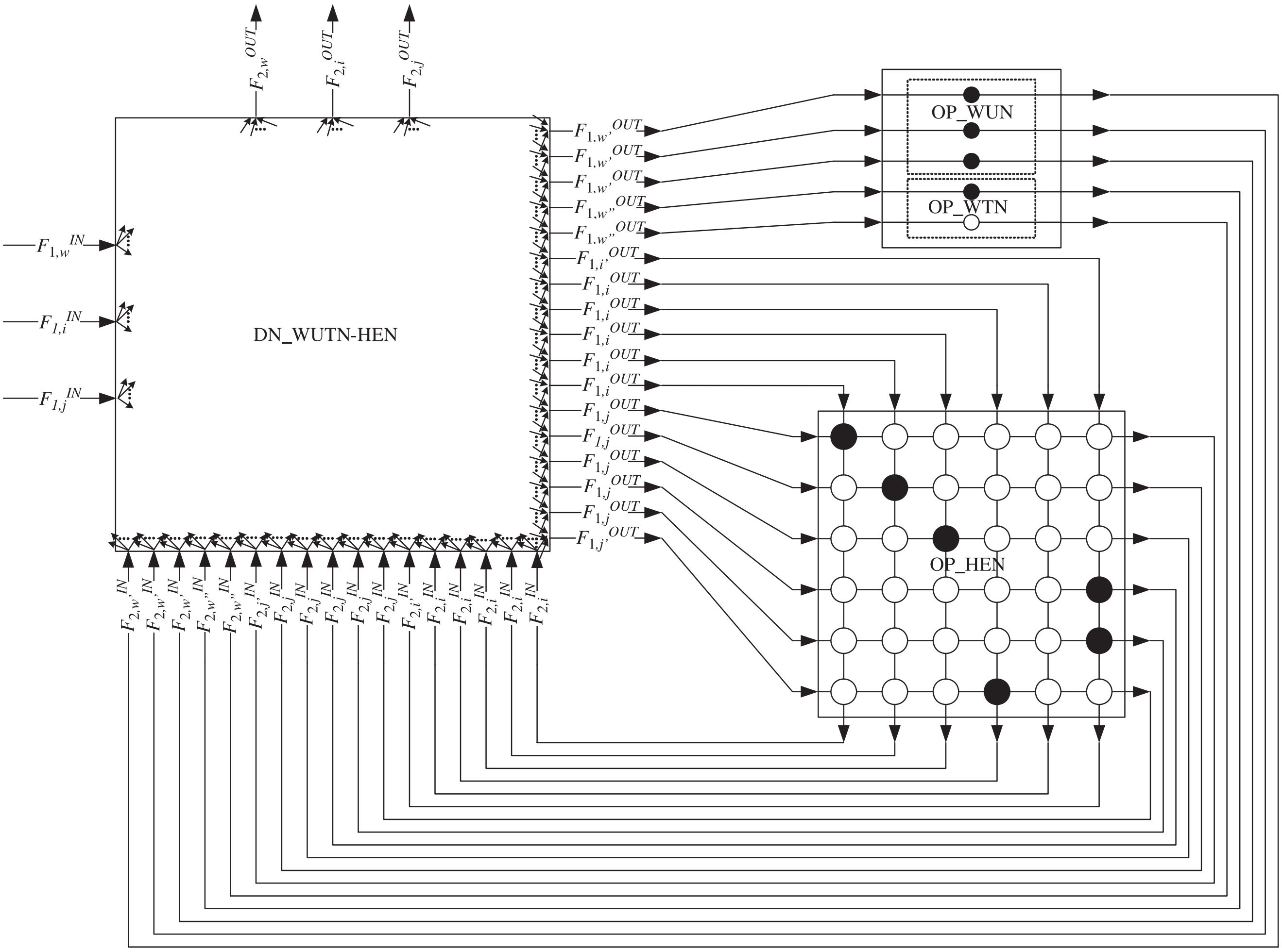

Fig. 7. State-space superstructure used for Case III in Example 2.

Table 3
A comparison between Cases I and II in Example 2

	Case I (sequential strategy)	Case II (simultaneous strategy)
TAC (USD yr^{-1})	2,742,198.4	2,631,805.4
Capital investment (USD yr^{-1})	406,290.8	305,913.3
Freshwater consumption rate ($\mathrm{kg\,s}^{-1}$)	77.3	87.2
Cold utility consumption rate (kW)	491	0
Hot utility consumption rate (kW)	3736.2	3671.4
Equipment requirements	2 heaters, 1 cooler, 4 heat exchangers	2 heaters, 0 cooler, 2 heat exchangers

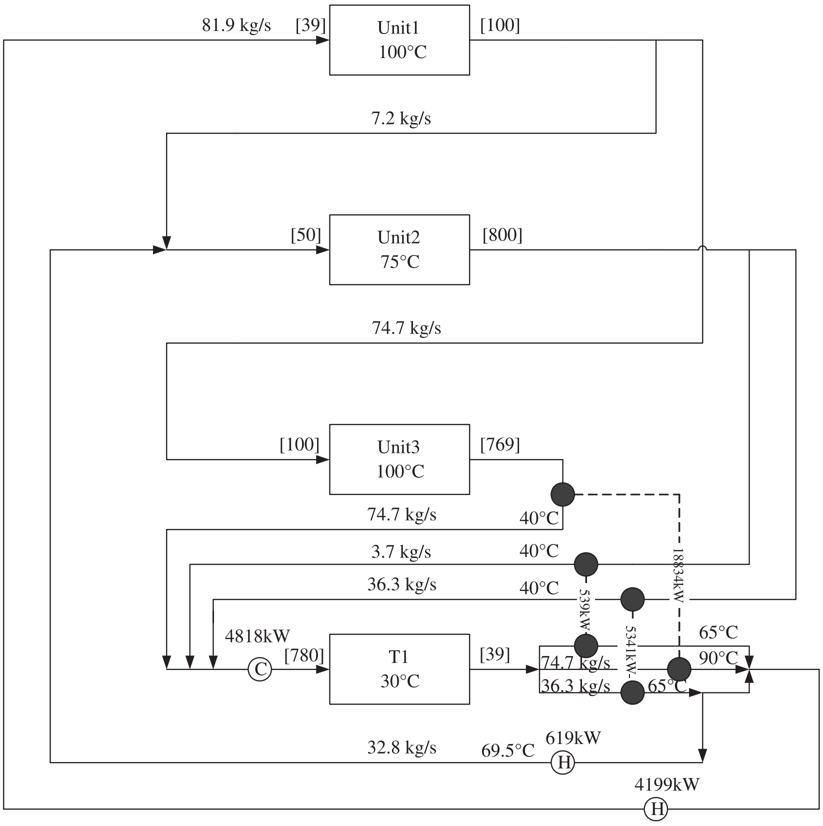

Fig. 8. Optimal WAHEN design for Case III in Example 2.

mixers are connected in the DN block, the connecting branches are not shown in this figure for the sake of legibility. The labels OP_WUN and OP_WTN are used to represent the process operators for water-using and wastewater-treatment networks, respectively, while OP_HEN is used to denote the operator for HEN. The darkened circles are the units eventually chosen in the optimal design. By including the aforementioned wastewater-treatment options in the state-space superstructure and solving the resulting model, an optimal WAHEN design can be obtained (see Fig. 8). Notice that, other than the water-using units, there are one wastewatertreatment unit, four heat exchangers, one cooler and two heaters in this network. Notice also that freshwater is not consumed in this system and the wastewater discharged rate is zero. The corresponding minimum TAC was found to be $6,555,774.1\,\mathrm{USD\,yr}^{-1}$, which consists of an annualized capital investment of $410,069.6\,\mathrm{USD\,yr}^{-1}$, a utility cost of $2,727,386.2\,\mathrm{USD\,yr}^{-1}$ and a treatment cost of $3418318.3\,\mathrm{USD\,yr}^{-1}$. The consumption rates of the cold and hot utilities (LP steam) needed in this case are 4818.6 and 4818.6 kW, respectively.

The last case study (Case IV) is performed for the purpose of demonstrating the impacts of wastewater-treatment units. In the present case, the concentration constraint imposed at the sink is the same as that adopted in Case III. Under this condition, a WAHEN is synthesized on the basis of a superstructure in which all treatment options are *excluded*. The resulting optimal network structure is shown in Fig. 9. Notice that there are two heat exchangers and two heaters in this design. Its TAC and the corresponding capital investment can be found to be 47,590,045.426 and $305,913.3\,\mathrm{USD\,yr}^{-1}$, respectively. The freshwater flow rate in this case is $4250\,\mathrm{kg\,s}^{-1}$, while the consumption rate of hot utility (LP steam) is 3671.4 kW. A comparison of the key features of the designs obtained in Cases III and IV is presented in Table 4.

5.3. Example 3

Let us finally consider the multicontaminant process data given in Table 5. Notice that these data were originally used by Mann and Liu (1999) for water-network synthesis only. The temperatures in this table are added in the present example to facilitate WAHEN design. By constructing the state-space superstructure and solving

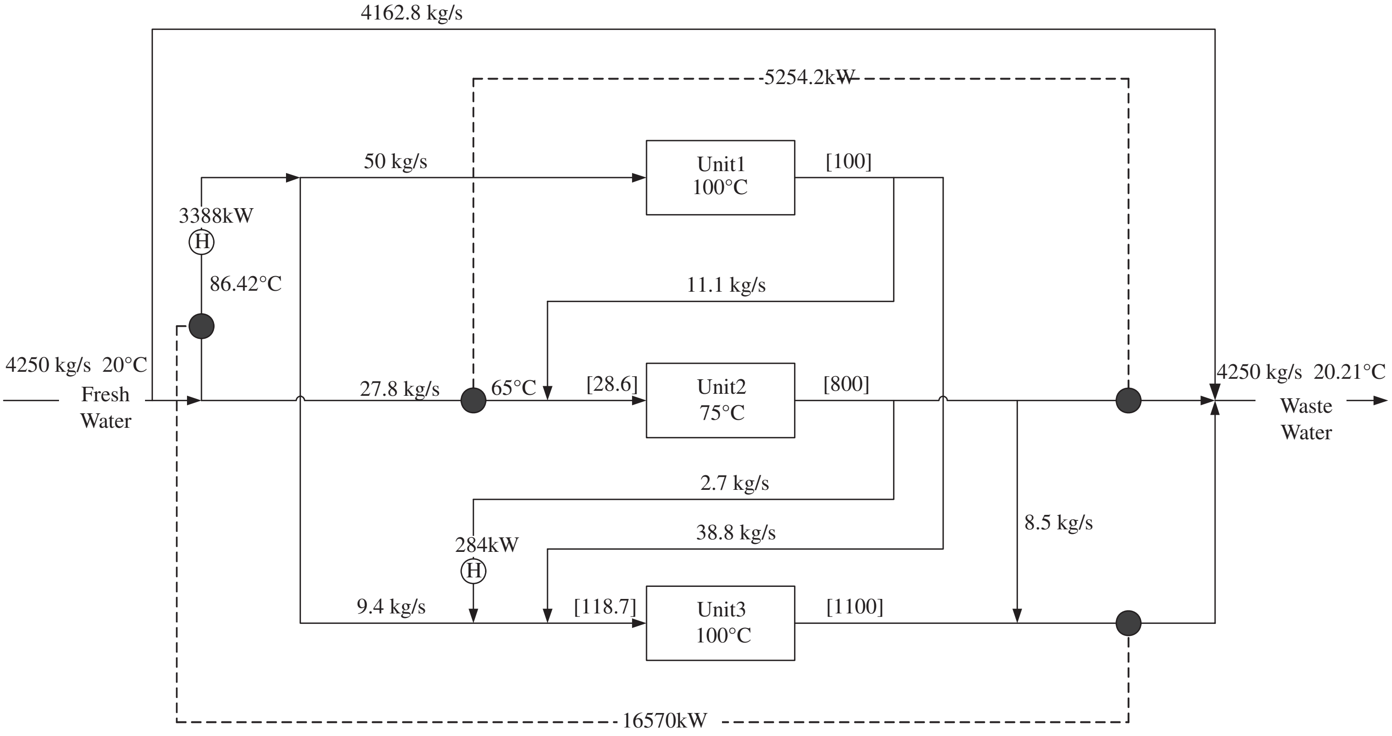

Fig. 9. Optimal WAHEN design for case IV in Example 2.

Table 4
A comparison between Cases III and IV in Example 2

	Case III (with treatment units)	Case IV (without treatment units)
TAC (USD yr^{-1})	6,555,774.1	47,590,645.4
Capital investment (USD yr^{-1})	410,069.6	305,913.3
Freshwater consumption rate (kg s^{-1})	0	4250
Cold utility consumption rate (kW)	4,818.6	0
Hot utility consumption rate (kW)	4,818.6	3671.4
Treatment cost (USD yr^{-1})	3,418,318.3	0
Equipment requirements	2 heaters, 1 cooler, 3 heat exchangers	2 heaters, 0 cooler, 2 heat exchangers

Table 5
Process data of Example 3

Unit (u)	Contaminant (s)	$\Delta m_{u,s}$(g s^{-1})	$\bar{C}^{\mathrm{in}}_{u,s}$(mg l^{-1})	$\bar{C}^{\mathrm{out}}_{u,s}$ (mg l^{-1})	$\bar{T}_u$(°C)
1	A	3.0	0	100	100
	B	2.4	0	80	
	C	1.8	0	60	
2	A	4.0	50	150	75
	B	3.0	40	115	
	C	3.6	15	105	
3	A	1.5	50	125	35
	B	0.6	50	80	
	C	2.0	30	130	

Temperature of secondary water=80 °C; maximum wastewater temperature =60° C.

the resulting MINLP, one can then generate the optimal structure in Fig. 10. It can be observed that this network is assembled with two heat exchangers, three coolers and one heater. From the optimal solution of the proposed model, the minimum TAC and the corresponding capital cost can also be obtained, i.e., 2,905,307.4 and $173,627.4$ USD yr^{-1}. In this design, the consumption rates of secondary water, and the cold and hot utilities (LP steam) can be determined to be 70 kg s^{-1}, 7140 and 1260 kW, respectively. On the basis of the designs produced in this example, it can be concluded that the proposed method is indeed suitable for applications in multicontaminant systems. In fact, this issue has never been properly addressed in any of the previous studies

6. Conclusions

The state-space superstructure has been modified in this study to formulate a MINLP model for one-step optimization of WAHEN designs with single- or multi-contaminant water streams. The advantage of this approach is that all possible design options, e.g., the wastewater-treatment units, the direct and indirect heat exchangers, can be easily incorporated in the model formulation. A hybrid optimization strategy has also been developed in this work to guarantee the solution quality and efficiency By interactively applying the deterministic and stochastic search techniques in this strategy, the global optimum can almost always be identified in all case studies presented in this paper.

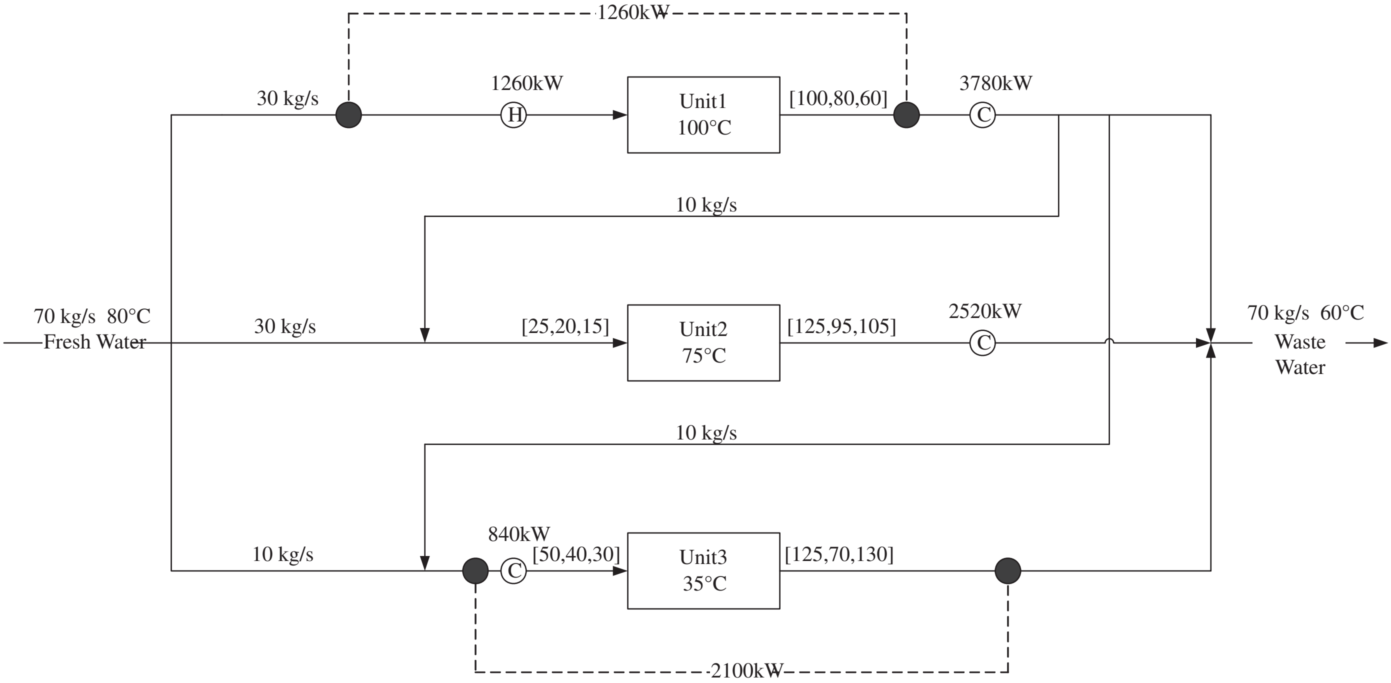

Fig. 10. Optimal WAHEN design in Example 3.

Notation

$A_{i,j}$	the heat-transfer area in an heat exchanger between the ith hot stream and jth cold stream
$F^{\mathrm{IN}}_{p,i}, F^{\mathrm{IN}}_{p,j}$	the products of heat capacity and mass flow rate of the ith hot stream and jth cold stream entering DN block from environment $(p=1)$ and from OP block $(p=2)$, respectively
$F^{\mathrm{OUT}}_{p,i}, F^{\mathrm{OUT}}_{p,j}$	the products of heat capacity and mass flow rate of the ith hot stream and jth cold stream leaving from DN block to the OP block $(p=1)$ and to the environment $(p=2)$, respectively
$f_{p,q,r}$	product of heat capacity and mass flow rate associated with a branch from the splitter on the qth hot, cold or water stream entering from environment $(p=1)$ and from OP block $(p=2)$, respectively, to the rth outlet mixer
$M_{\mathrm{ext}}, N_{\mathrm{ext}}$	the numbers of exterior junctions on the DN block for the hot and cold streams, respectively, from (or to) the environment
$M_{\mathrm{int}}, N_{\mathrm{int}}$	the numbers of interior junctions on the DN block for the hot and cold streams, respectively, from (or to) the OP block
$M^{\mathrm{IN}}_{p}, N^{\mathrm{IN}}_{p}$	the numbers of inlet splitters for hot and cold streams on the DN block from environment $(p=1)$ and from OP block $(p=2)$, respectively
$M^{\mathrm{OUT}}_{p}, N^{\mathrm{OUT}}_{p}$	the numbers of outlet mixers for hot and cold streams on the DN block to the OP block $(p=1)$ and to the environment $(p=2)$, respectively
m_i, n_j	the numbers of interior junctions associated with exterior hot stream i and exterior cold stream j, respectively
m, n	the numbers of interior junctions associated with hot streams and cold streams in general
$T^{\mathrm{in}}_{w}, T^{\mathrm{out}}_{w}$	the water-stream temperatures at the inlet and outlet of water using unit and treatment unit (w), respectively
$T^{\mathrm{in}}_{i}, T^{\mathrm{out}}_{i}$	the hot-stream temperatures at the inlet and outlet of exchanger (i,j), respectively
$T^{\mathrm{in}}_{j}, T^{\mathrm{out}}_{j}$	the cold-stream temperatures at the inlet and outlet of exchanger (i,j), respectively
$T^{\mathrm{IN}}_{p,i}, T^{\mathrm{IN}}_{p,j}, T^{\mathrm{IN}}_{p,w}$	the temperatures of the ith hot stream, jth cold stream and water streams entering DN block from environment $(p=1)$ and from OP block $(p=2)$, respectively
$T^{\mathrm{OUT}}_{p,i}, T^{\mathrm{OUT}}_{p,j}, T^{\mathrm{OUT}}_{p,w}$	the temperatures of the ith hot stream, jth cold stream and water streams leaving from DN block to the OP block $(p=1)$ and to the environment $(p=2)$, respectively
$\Delta\overline{T}_{i,j}$	the log-mean temperature difference in the exchanger (i,j)
$\Delta T_{\min}$	the minimum temperature approach
$U_{i,j}$	the overall heat-transfer coefficient of exchanger (i,j)
$z_{i,j}$	the binary variable reflecting whether or not the match between streams i and j exists

Greek letters

δ	the range of perturbation interval
$\varepsilon_{p,q,r}$	the randomly generated perturbation for $\varphi_{p,q,r}$
$\Gamma_H, \Gamma_C, \Gamma_W$	the sets of hot, cold and water streams entering the OP block

$\varphi_{p,q,r}$	the split ratio of a branch leaving the splitter on the qth hot (or cold) stream entering the DN block from environment ($p=1$) and from OP block ($p=2$), respectively, to the rth mixer leaving the DN block

Subscripts

ext	external
int	internal

Superscripts

in	exchanger inlet
out	exchanger outlet
IN	DN inlet
OUT	DN outlet

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