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Global Superstructure Optimization for the Design of Integrated Process Water Networks

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We propose a general superstructure and a model for the global optimization for integrated process water networks. The superstructure consists of multiple sources of water, water-using processes, wastewater treatment, and pre-treatment operations. Unique features are that all feasible interconnections are considered between them and multiple sources of water can be used. The proposed model is formulated as a nonlinear programing (NLP) and as a mixed integer nonlinear programing (MINLP) problem for the case when 0–1 variables are included for the cost of piping and to establish optimal trade-offs between cost and network complexity. To effectively solve the NLP and MINLP models to global optimality we propose tight bounds on the variables, which are expressed as general equations. We also incorporate the cut proposed by Karuppiah and Grossmann to significantly improve the strength of the lower bound for the global optimum. The proposed model is tested on several examples. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 434–457, 2011
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Introduction

The process industry consumes a large amount of water. For instance, water is used for washing operations, separation processes, steam and power generation, cooling, etc. These processes in turn generate wastewater, which is usually processed in treatment units before discharge to the environment. The shortage of freshwater, its increasing cost, and one of the treatment processes, as well as strict environmental regulations on the industrial effluents, provide a strong motivation for developing approaches and techniques to design more efficient process water networks.

The two major approaches for the optimal design of water network systems are water pinch technology and mathematical programing. A comprehensive review of these approaches, as well as systematic methods of chemical process design, are given by Rossiter,[2] El-Halwagi,[3] Biegler et al.,[4] Mann and Liu,[5] Bagajewicz,[6] Jėzowski,[7] Bagajewicz and Faria,[8] and Foo.[9]

Water pinch technology relies on graphic representations and it is based on an extension of pinch analysis technique for heat integration.[10] The first authors, who introduced the notion of synthesizing mass-exchange networks (MEN's), were El-Halwagi and Manousiouthakis.[11,12] They considered mass exchange between rich and lean process streams. After that, a targeting approach for minimum freshwater consumption was developed by Wang and Smith[13–15] and later extended and improved by a number of researchers.[9,16–24]

The mathematical programing approach is based on the optimization of a superstructure. The seminal article addressed a mathematical programing formulation of water network was given by Takama et al.[25] They considered a system consisting of water-using and wastewater-treating units. In addition to this, they generated a superstructure of

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all possible re-use and regeneration opportunities and formulated the problem of optimal water allocation in a petroleum refinery as a nonlinear programing (NLP) problem. After their article the solution of the mathematical programing formulation for this problem was not addressed for many years.[6] In many articles, the total water network is decomposed into two parts (network with water-using operations and wastewater treatment network) which are solved separately. For example, Kuo and Smith[18] presented an extension of the methodology for the design of distributed effluent treatment systems previously given by Wang and Smith.[14] They presented an improved method for targeting the treatment flowrate and the distribution of load between multiple treatment processes. In addition to this, Galan and Grossmann[26] addressed the optimal design of distributed wastewater network where multiple contaminants are considered. They proposed a heuristic search procedure based on the successive solution of a relaxed linear model and the original nonconvex nonlinear model. Their procedure has the capability of finding global or near global optimum solutions. In addition, the model was extended for selecting different treatment technologies for handling membrane separation modules. Savelski and Bagajewicz[27,28] developed necessary optimality conditions (maximum outlet concentrations from water-using units and concentration monotonicy) for single and multiple water allocation systems in refineries and process plants. They used these conditions to eliminate the nonlinearities in the water network models arising in the mass balance equations in the form of bilinear terms (concentration times flowrate). According to this, they showed that the nonlinear model of water networks for single component can be linearized. Quesada and Grossmann[29] proposed a rigorous procedure for the global optimization of bilinear process networks with multicomponent streams. Their procedure is based on a reformulation-linearization technique applied to nonlinear models to obtain a relaxed linear programing formulation that provides a valid lower bound to the global optimum. Castro et al.[30] proposed the two-stage solution strategy for the optimal design of distributed wastewater networks with multiple contaminants. In the first stage, a decomposition method is used that replaces the nonlinear program by a succession of linear programs, one for each treatment unit. In the second stage, the resulting network is used as a starting point for the solution of the nonlinear model with a local optimization solver.

The problem of designing the total water networks has been addressed in relatively few articles.[7] Doyle and Smith[17] proposed a method based on NLP for targeting maximum water reuse in processing systems. To overcome the difficulties associated with the nonlinear optimization model, they used a linear model to provide an initialization for the nonlinear model. Alva-Argáez et al.[31] proposed an integrated methodology for the design of industrial water systems. Their decomposition strategy is based on a recursive procedure where the original mixed-integer nonlinear problem (MINLP) is replaced by a sequence of mixed-integer linear problems (MILPs). Huang et al.[32] proposed a mathematical model for determining the optimal water usage and treatment network in chemical plants. They presented a modified version of the superstructure proposed by Takama et al.[25] and included in the model design equations of all wastewater treatment facilities and all units, which use either process or utility water so that better integration on a plan-wide scale can be achieved. Feng and Seider[33] proposed a network structure in which internal water mains are used. Their structure simplifies the piping network as well as the operation and control of large plants involving many water-using processes. Gunaratnam et al.[34] presented an automated design of total water systems where the optimal distribution of water to satisfy process demands and optimal treatment of effluent streams are considered simultaneously. They used a two-stage optimization approach to solve the MINLP model involving an MILP in the first stage to initialize the problem. In the second stage, the design is fine-tuned using MINLP. In addition to this, the network complexity is controlled by specifying the minimum permissible flowrates in the network. Their methodology provides a robust technique but it does necessarily yield the global optimum.

Karuppiah and Grossmann[1] addressed the problem of optimal synthesis of an integrated water system consisting of water-using processes and water treatment operations. In contrast to previous work, they proposed a spatial branch and contract algorithm for the rigorous global optimization of the nonlinear program of the integrated water system. In their algorithm, tight lower bounds on the global optimum are obtained by solving a relaxation of the original problem obtained by approximating the nonconvex terms in the model with piecewise linear estimators. Li and Chang[35] developed an efficient initialization strategy to solve the NLP and MINLP models for water network with multiple contaminants. In the MINLP model, they formulated structural constraints to manipulate structural complexity, but global optimality is not guaranteed. Also, they reported that the optimum solution obtained by the initialization strategy is at least as good as results reported in the literature but with less computation time to achieve convergence. In the same year, Alva-Argaez et al.[36] proposed a systematic approach to address water reuse in oil refineries. The methodology is based on the water-pinch decomposition. Their approach simplifies the challenges of the optimization problem making systematic use of water-pinch insights to define successive projections in the solution space.

Putra and Amminudin[37] proposed an alternative solution strategy for solving the total water system design problem by using the MILP and NLP in a two-step optimization approach. Their approach, which is not guaranteed to find the global optimum, has the capability of generating multiple optimal solutions and to handle practical considerations, as well as to provide users with the ability to control water network during the optimization process. Luo and Uan[38] presented a superstructure-based method for the optimization of integrated water systems with the heuristic particle swarm optimization (PSO) algorithm. Karuppiah and Grossmann[39] presented a formulation for representing and optimizing integrated water networks operating under uncertain conditions of the contaminant loads in the process units and contaminant removals of the treatment units. They formulated a multi-scenario nonconvex MINLP model for globally optimizing an integrated water network operating under uncertainty. Further, they proposed a spatial branch and cut algorithm combining the concepts of Lagrangean relaxation and convex relaxation to generate strong bounds for the global optimum.

Notice that in the previously mentioned articles the vast majority are based on linearization of the nonlinear models, or use linear models to provide an initialization for the nonlinear models, which are solved with local optimization solvers. Moreover, a number of authors replace the MINLP problems by a sequence of the MILPs. Bagajewicz and Faria[8] and Faria and Bagajewicz[40] presented the evolution of the water network allocation problem given by Takama et al.[25] In addition, they included the water pre-treatment subsystem in the network and discussed the end-of-pipe wastewater treatment and the complete water integration.

It should be mentioned that the problem of designing total water networks has been addressed in relatively few articles due to its complexity.[7] The main complexity in the nonlinear model is due to the bilinear terms in the mass balance equations (flowrate times concentration) and the concave cost terms in the objective function with which the solution for the total water network is not guaranteed to be the global optimum. In addition to this, it is worth pointing out that in the majority of the published articles all possible options are not considered in the total water network such as all feasible interconnections in the network, multiple sources of water of different quality, pre-treatment of the water, mass transfer and non-mass transfer water-using operations. Moreover, in many articles the cost of water pumping through pipes and the investment cost for pipes are not included in the objective function. However, there are also water network models that incorporate piping costs in the form of linear and nonlinear models.[31,34,39] For example, Gunaratnam et al.[34] assume fixed velocity of the flows and model the cost of piping as linear cost function with fixed charge. In contrast, Karuppiah and Grossmann[39] assume a concave cost function with fixed charge. The more rigorous model that optimizes diameters and pressure drops to account for the trade-off between pumping and investment costs has not been considered to our knowledge.

The main objective of this article is to propose a general superstructure and a global optimization approach for the design of integrated process water networks. The superstructure consists of multiple sources of water, water-using (mass transfer and non-mass transfer) processes, water treatment operations, and all feasible interconnections in the network. We propose nonconvex NLP and MINLP models for the integrated water network. We also develop bounds on the variables as general equations obtained by physical inspection of the superstructure and use logic specifications that have the capability of reducing the feasible region, and helping global NLP and MINLP solvers to find more efficiently the global optimum. In the MINLP model, we include the costs of piping (concave function of the flowrate with fixed charge) and the costs of water pumping through pipes (linear function of the flowrate). With the proposed model we can also establish the trade-offs between network cost and network complexity in terms of number of pipe connections. Although all the problems in this article are solved to global optimality, we also describe a two-stage solution method in which we first solve the relaxed MINLP model to fix a subset of 0–1 variables to zero so as to solve a reduced size MINLP for which its optimality gap can be readily established. Several examples, including large-scale industrial problems, are presented in the article to illustrate the proposed method. We use the general purpose global optimization solver BARON[41] to solve the proposed models to global optimality.

The outline of the article is as follows. First, we present the problem statement. We then introduce the general water network superstructure, followed by its mathematical formulation. We then discuss the solution approach for solving large-scale industrial MINLP problems. The computational results and discussion are given in the following section. Finally, in the last section, we present general conclusions.

Problem Statement

The problem addressed in this article can be stated as follows. Given is a set of single/multiple water sources with/without contaminants, a set of water-using units and wastewater treatment operations, fixed water demands of process units, maximum concentrations of contaminants in inlet streams at process units, mass loads of contaminants in process units, the costs of water sources and wastewater treatment units, percent removal of each contaminant in treatment units, and the maximum contaminant concentrations in the discharge effluent to the environment. The problem consists in determining the interconnections, flowrates, and contaminants concentration of each stream in the water network, the freshwater consumption and wastewater generation, and the total annual cost of the water network (costs of freshwater consumption, wastewater treatment, piping network, pumping water through pipes in the network).

The proposed model is based on the following assumptions: the number of water sources is fixed, the number of water-using and water treatment operations is fixed, the flowrates through the water-using process operations are usually assumed to be fixed but can also be treated as continuous variables to model mass transfer operations in the proposed model, the network operates under isothermal condition and isobaric conditions. We should note that the assumption of fixed flowrates can easily be relaxed as shown in Example 3 in the case when the inlet and outlet flowrates are different. In addition, we considered the water flowrate through the process unit to be a continuous variable determined by the optimization.

Superstructure of the Integrated Process Water Network

The proposed model of the integrated water network relies on the superstructure given in Figure 1. The superstructure, which is an extension and generalization of the one given by Karuppiah and Grossmann,[1] consists of one or multiple sources of water of different quality, water-using processes, and wastewater treatment operations. The unique feature is that all feasible connections are considered between them, including water re-use, water regeneration and re-use, water regeneration recycling, local recycling around process and treatment units, and pre-treatment of feedwater streams. Multiple sources of water include water of different quality that can be used in the various operations, and which may be sent first for pre-treatment. The superstructure incorporates both the mass transfer and non-mass transfer operations. In the

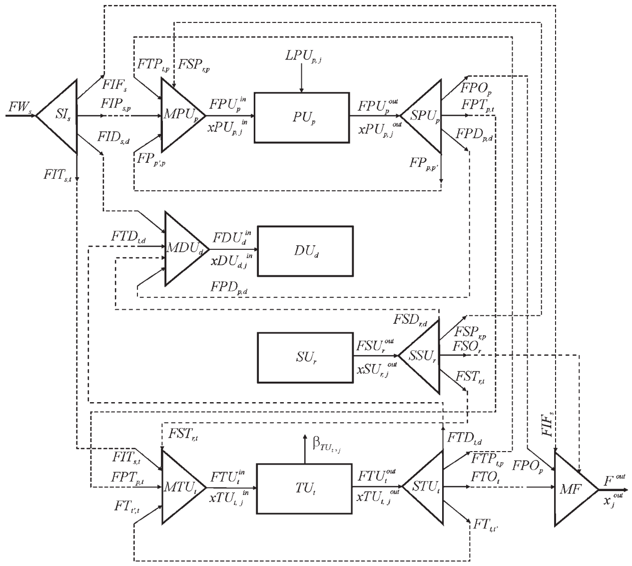

Figure 1. Generalized superstructure for the design of integrated process water networks.

mass transfer process operations there is direct contact, usually countercurrent, between a contaminant-rich process stream and a contaminant-lean water stream. These units can be represented as a "true" contaminant-rich process streams. In this case, during the mass-transfer process the contaminant loads $LPU_{p,j}$ are transferred from the process streams to the water. The contaminant concentration in the process stream is reduced, while the contaminant concentration increases in the water stream.[5]

In many processes, there is loss of water that cannot be re-used in a water-using operation. This unit represents a water demand unit or water sink. Cooling towers are typical process units where water is lost by evaporation. From some water-using operations water is available for re-use in other operations. These units represent water sources.

According to this, the superstructure can be used to represent separate subsystems as well as an integrated total system. Furthermore, it enables modeling different types of water network optimization problems as will be shown later in the article.

Mathematical Programing Models

The mathematical model of integrated process water networks consists of mass balance equations for water and the contaminants for every unit in the network. The model is formulated as a nonconvex NLP, and as a nonconvex mixed-integer nonlinear programing (MINLP) for the case when 0–1 variables are included to model the cost of piping and/or selection of technologies for treatment. The nonlinearities in the models appear in the mass balance equations in the form of bilinear terms (concentration times flowrate). In addition to this, nonlinearities appear in the objective function as concave terms of the cost functions for the water-treatment operations.

Hence, the water network models are nonconvex, and in most cases lead to multiple local solutions making it difficult to obtain the global or a near-global optimal solution. The basic options of the proposed water network optimization model are given as follows.

First of all, the model enables the choice of a single or multiple sources of water that are available for the network plant operation. Second, water sources can be clean water without contaminants or water with multiple contaminants. Water with higher quality is more expensive and the total cost will be minimized at the expense of lower quality water as shown later in illustrative examples. Water with contaminants on the other hand may be directly sent to treatment units before using it for water-using operations. Third, the water network can consist only of the water-using operations or wastewater treatment operations. In addition, it can be an integrated water network including both water-using operations and wastewater treatment operations. Fourth, all feasible interconnections are possible in the network for every option mentioned before. Fifth, it is possible to choose local recycles around the water-using operations or the wastewater treatment operations. Local recycling[15] can be used to satisfy the flowrate constraints and in these cases it is possible to have an additional reduction in water consumption as is shown later in an illustrative example. Sixth, as industrial water network systems usually consist of different types of water-using operations that can be classified as mass-transfer operations and non-mass transfer operations[15] both types of these operations are included in the superstructure. In addition to this, in many processes, there is loss of water that is not available for re-use in a water-using operation. Hence, this unit involves water demand unit and is a water sink. Moreover, from some water-using operations water is available for re-use in other operations and they represent sources of water. In all the aforementioned options, the number of contaminants, water sources, water-using operations, and wastewater treatment operations is fixed. To make the model more general, we also address to class of water network problems when the flowrate through process units is a continuous variable. It should be mentioned that in this case the feasible space is increased, and several additional bilinear terms are added for the water-using process units to the model, which can increase the computational requirements as will be shown later in the article. The proposed model enables modeling and optimization of any of the aforementioned options of the water network superstructure. Finally, it should be emphasized that some features of the proposed model (water consuming processes, self recycles, multiple water sources, etc.) are not usually included in other water network models reported in the literature.

Mathematical model

In this section, we propose an MINLP model for the superstructure given in Figure 1. It should be noted that this MINLP can be reduced to an NLP when 0–1 variables and corresponding mixed-integer and integer constraints are not included.

Initial splitters

The feedwater of an initial splitter SI_s for freshwater source $s \in SW$ can be clean water without contaminants or water with single/multiple contaminants. Freshwater from the initial splitter can be directed to the mixer process unit, the mixer treatment unit, the mixer demand units, or the final mixer. The connection between the initial splitter and the mixers in the network depends of the special network case that is considered. For instance, if we consider only multiple wastewater feeds and the wastewater distribution subsystem there will be connections between the initial splitter and the final mixer. However, in an integrated system consisting of water-using units and wastewater treatment units, connections between the initial splitter and the final mixer do not exist because it would lead to a loss of freshwater.

The overall material balance for the initial splitter is given by Eq. 1:

$$\mathrm{FW}_s = \mathrm{FIF}_s + \sum_{p\in \mathrm{PU}} \mathrm{FIP}_{s,p} + \sum_{d\in \mathrm{DU}} \mathrm{FID}_{s,d} + \sum_{t\in \mathrm{TU}} \mathrm{FIT}_{s,t} \quad \forall s \in \mathrm{SW}. \tag{1}$$

For each of the corresponding flowrates, upper and lower bound constraints are formulated in terms of the binary variables that denote the existence of the pipes of these streams.

$$\mathrm{FIF}_s^{\mathrm{L}} \cdot y_{\mathrm{FIF}_s} \le \mathrm{FIF}_s \le \mathrm{FIF}_s^{\mathrm{U}} \cdot y_{\mathrm{FIF}_s} \quad \forall s \in \mathrm{SW} \tag{2}$$

$$\mathrm{FIP}_{s,p}^{\mathrm{L}} \cdot y_{\mathrm{FIP}_{s,p}} \le \mathrm{FIP}_{s,p} \le \mathrm{FIP}_{s,p}^{\mathrm{U}} \cdot y_{\mathrm{FIP}_{s,p}} \quad \forall s \in \mathrm{SW}, \forall p \in \mathrm{PU} \tag{3}$$

$$\mathrm{FID}_{s,d}^{\mathrm{L}} \cdot y_{\mathrm{FID}_{s,d}} \le \mathrm{FID}_{s,d} \le \mathrm{FID}_{s,d}^{\mathrm{U}} \cdot y_{\mathrm{FID}_{s,d}} \quad \forall s \in \mathrm{SW},\ \forall d \in \mathrm{DU} \tag{4}$$

$$\mathrm{FIT}_{s,t}^{\mathrm{L}} \cdot y_{\mathrm{FIT}_{s,t}} \le \mathrm{FIT}_{s,t} \le \mathrm{FIT}_{s,t}^{\mathrm{U}} \cdot y_{\mathrm{FIT}_{s,t}} \quad \forall s \in \mathrm{SW}, \forall t \in \mathrm{TU}. \tag{5}$$

Mixer process units

The mixer process unit MPU_p consists of a set of inlet streams from the splitter source unit, the splitter treatment unit, the initial splitter, and the splitter process unit. An outlet stream from the mixer process unit is directed to the process unit. The overall material balance for the mixer process unit is given by Eq. 6 and the mass balance for each contaminant j by Eq. 7, which involves bilinear terms:

$$\mathrm{FPU}_p^{\mathrm{in}} = \sum_{r\in \mathrm{SU}} \mathrm{FSP}_{r,p} + \sum_{t\in \mathrm{TU}} \mathrm{FTP}_{t,p} + \sum_{s\in \mathrm{SW}} \mathrm{FIP}_{s,p} + \sum_{\substack{p'\in \mathrm{PU}\\ p\neq p', R_p=0}} \mathrm{FP}_{p',p} + \sum_{\substack{p'\in \mathrm{PU}\\ R_p=1}} \mathrm{FP}_{p',p}, \quad \forall p \in \mathrm{PU} \tag{6}$$

$$\mathrm{FPU}_p^{\mathrm{in}} \cdot x\mathrm{PU}_{p,j}^{\mathrm{in}} = \sum_{r\in \mathrm{SU}} \mathrm{FSP}_{r,p} \cdot x\mathrm{SU}_{r,j}^{\mathrm{out}} + \sum_{t\in \mathrm{TU}} \mathrm{FTP}_{t,p} \cdot x\mathrm{STU}_{t,j}^{\mathrm{out}} + \sum_{s\in \mathrm{SW}} \mathrm{FIP} \cdot xW_{s,j}^{\mathrm{in}} + \sum_{\substack{p'\in \mathrm{PU}\\ p\neq p', R_p=0}} \mathrm{FP}_{p',p} \cdot x\mathrm{SPU}_{p',j}^{\mathrm{out}} + \sum_{\substack{p'\in \mathrm{PU}\\ R_p=1}} \mathrm{FP}_{p',p} \cdot x\mathrm{SPU}_{p',j}^{\mathrm{out}}, \quad \forall p \in \mathrm{PU},\ \forall j. \tag{7}$$

Process units

The process unit PU_p consists of an inlet stream $\mathrm{FPU}_p^{\mathrm{in}}$ from the mixer process unit and an outlet stream $\mathrm{FPU}_p^{\mathrm{out}}$ from the process unit. The inlet and outlet water flows for the process unit are equal. The overall material balance is given by Eq. 8 and the mass balance equation for each contaminant j by Eq. 9:

$$\mathrm{FPU}_p^{\mathrm{in}} = \mathrm{FPU}_p^{\mathrm{out}} \quad \forall p \in \mathrm{PU} \tag{8}$$

$$\mathrm{FPU}_p^{\mathrm{in}} \cdot x\mathrm{PU}_{p,j}^{\mathrm{in}} + \mathrm{LPU}_{p,j} = \mathrm{FPU}_p^{\mathrm{out}} \cdot x\mathrm{PU}_{p,j}^{\mathrm{out}} \quad \forall p \in \mathrm{PU}, \forall j. \tag{9}$$

When the flowrate is assumed to be fixed $\mathrm{FPU}_p^{\mathrm{in}}$ is constant. Otherwise, it is treated as a continuous variable.

The outlet concentrations in the flows from the process units and the inlet concentrations to the splitter process units are the same as shown in Eq. 10:

$$x\mathrm{PU}_{p,j}^{\mathrm{out}} = x\mathrm{SPU}_{p,j}^{\mathrm{in}} \quad \forall p \in \mathrm{PU},\ \forall j. \tag{10}$$

Splitter process units

The splitter process unit SPU_p consists of an inlet stream from the process unit, and a set of outlet streams directed to the final mixer, the mixer treatment unit, the mixer demand unit, and the mixer process unit. The overall material balance for the splitter process unit is given by Eq. 11:

$$\mathrm{FPU}_p^{\mathrm{out}} = \mathrm{FPO}_p + \sum_{t\in \mathrm{TU}} \mathrm{FPT}_{p,t} + \sum_{d\in \mathrm{DU}} \mathrm{FPD}_{p,d} + \sum_{\substack{p'\in \mathrm{PU}\\ p\neq p', R_p=0}} \mathrm{FP}_{p',p} + \sum_{\substack{p'\in \mathrm{PU}\\ R_p=1}} \mathrm{FP}_{p',p} \quad \forall p \in \mathrm{PU}. \tag{11}$$

The contaminant concentration of every stream leaving the splitter is equal to the contaminant concentration of the inlet stream and this equality is given by Eq. 12:

$$x\mathrm{SPU}_{p,j}^{\mathrm{out}} = x\mathrm{SPU}_{p,j}^{\mathrm{in}} \quad \forall p \in \mathrm{PU},\ \forall j. \tag{12}$$

The lower and upper bound constraints that relate the 0–1 variables with the flows between the splitter process units and all mixers in the network are given as follows.

$$\mathrm{FPO}_p^{\mathrm{L}} \cdot y_{\mathrm{FPO}_p} \le \mathrm{FPO}_p \le \mathrm{FPO}_p^{\mathrm{U}} \cdot y_{\mathrm{FPO}_p} \quad \forall p \in \mathrm{PU} \tag{13}$$

$$\mathrm{FPT}_{p,t}^{\mathrm{L}} \cdot y_{\mathrm{FPT}_{p,t}} \le \mathrm{FPT}_{p,t} \le \mathrm{FPT}_{p,t}^{\mathrm{U}} \cdot y_{\mathrm{FPT}_{p,t}} \quad \forall p \in \mathrm{PU}, \forall t \in \mathrm{TU} \tag{14}$$

$$\mathrm{FPD}_{p,d}^{\mathrm{L}} \cdot y_{\mathrm{FPD}_{p,d}} \le \mathrm{FPD}_{p,d} \le \mathrm{FPD}_{p,d}^{\mathrm{U}} \cdot y_{\mathrm{FPD}_{p,d}} \quad \forall p \in \mathrm{PU},\ \forall d \in \mathrm{DU} \tag{15}$$

$$\mathrm{FP}_{p',p}^{\mathrm{L}} \cdot y_{\mathrm{FP}_{p',p}} \le \mathrm{FP}_{p',p} \le \mathrm{FP}_{p',p}^{U} \cdot y_{\mathrm{FP}_{p',p}} \quad \forall p \in \mathrm{PU}, \forall p' \in \mathrm{PU},\ p' \neq p, R_p = 0 \tag{16}$$

$$\mathrm{FP}_{p',p}^{\mathrm{L}} \cdot y_{\mathrm{FP}_{p',p}} \le \mathrm{FP}_{p',p} \le \mathrm{FP}_{p',p}^{U} \cdot y_{\mathrm{FP}_{p',p}} \quad \forall p \in \mathrm{PU}, \forall p' \in \mathrm{PU}, R_p = 1. \tag{17}$$

Demand and source process units

The demand process unit is shown in Figure 2. The mixer demand unit MDU_d unit consists of a set of inlet streams

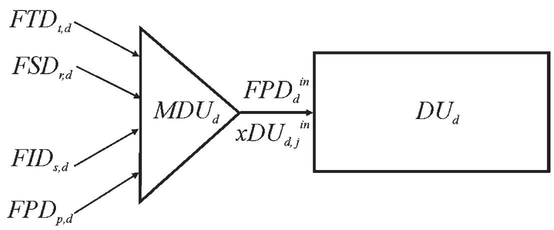

Figure 2. Demand process unit.

from the splitter treatment unit, the splitter source unit, initial splitter, and the splitter process unit. An outlet stream from the mixer demand unit is directed to the demand unit.

The overall material balance for the mixer demand unit is given by Eq. 18 and the mass balance for each contaminant j by Eq. 19:

$$\begin{aligned} \mathrm{FDU}_d^{\mathrm{in}} = \sum_{t\in \mathrm{TU}} \mathrm{FTD}_{t,d} + \sum_{r\in \mathrm{SU}} \mathrm{FSD}_{r,d} + \sum_{s\in \mathrm{SW}} \mathrm{FID}_{s,d} \\ + \sum_{p\in \mathrm{PU}} \mathrm{FPD}_{p,d} \qquad \forall d \in \mathrm{DU} \end{aligned} \tag{18}$$

$$\begin{aligned} \mathrm{FDU}_d^{\mathrm{in}} \cdot x\mathrm{SDU}_{d,j}^{\mathrm{in}} = \sum_{t\in \mathrm{TU}} \mathrm{FTD}_{t,d} \cdot x\mathrm{STU}_{t,j}^{\mathrm{out}} \\ + \sum_{r\in \mathrm{SU}} \mathrm{FSD}_{r,d} \cdot x\mathrm{SU}_{r,j}^{\mathrm{out}} + \sum_{s\in \mathrm{SW}} \mathrm{FID}_{s,d} \cdot xW_{s,j}^{\mathrm{in}} + \\ + \sum_{p\in \mathrm{PU}} \mathrm{FPD}_{p,d} \cdot x\mathrm{SPU}_{p,j}^{\mathrm{out}} \qquad \forall d \in \mathrm{DU},\ \forall j. \end{aligned} \tag{19}$$

In addition, the contaminant concentration at the demand inlet has to be less or equal to the maximum allowed contaminant concentration:

$$x\mathrm{SDU}_{d,j}^{\mathrm{in}} \le x\mathrm{SDU}_{d,j}^{\mathrm{in,max}} \quad \forall d \in \mathrm{DU},\ \forall j\,. \tag{20}$$

The source process unit is shown in Figure 3. The splitter source unit SSU_r unit consists of an inlet stream from the source unit and a set of outlet streams directed to the mixer process unit, the final mixer, the mixer treatment unit, and the mixer demand unit.

The overall material balance for the splitter source unit is given by Eq. 21. Notice, that the contaminant concentration at the outlet of the source unit and the outlet of the splitter source unit is the same.

$$\begin{aligned} \mathrm{FSU}_r^{\mathrm{out}} = \sum_{p\in \mathrm{PU}} \mathrm{FSP}_{r,p} + \mathrm{FSO}_r + \sum_{t\in \mathrm{TU}} \mathrm{FST}_{r,t} \\ + \sum_{d\in \mathrm{DU}} \mathrm{FSD}_{r,d} \qquad \forall r \in \mathrm{SU}\,. \end{aligned} \tag{21}$$

The lower and upper bound constraints that relate the flows and 0–1 variables for the streams between the splitter source units and all mixers in the network are given as follows.

$$\mathrm{FSP}_{r,p}^{\mathrm{L}} \cdot y_{\mathrm{FSD}_{r,p}} \le \mathrm{FSP}_{r,p} \le \mathrm{FSP}_{r,p}^{\mathrm{U}} \cdot y_{\mathrm{FSP}_{r,p}} \quad \forall r \in \mathrm{SU},\ \forall p \in \mathrm{PU} \tag{22}$$

$$\mathrm{FSO}_r^{\mathrm{L}} \cdot y_{\mathrm{FSO}_r} \le \mathrm{FSO}_r \le \mathrm{FSO}_r^{\mathrm{U}} \cdot y_{\mathrm{FSO}_r} \quad \forall r \in \mathrm{SU} \tag{23}$$

$$\mathrm{FST}_{r,t}^{\mathrm{L}} \cdot y_{\mathrm{FST}_{r,t}} \le \mathrm{FST}_{r,t} \le \mathrm{FST}_{r,t}^{\mathrm{U}} \cdot y_{\mathrm{FST}_{r,t}} \quad \forall r \in \mathrm{SU}, \forall t \in \mathrm{TU} \tag{24}$$

$$\mathrm{FSD}_{r,d}^{\mathrm{L}} \cdot y_{\mathrm{FSD}_{r,d}} \le \mathrm{FSD}_{r,d} \le \mathrm{FSD}_{r,d}^{\mathrm{U}} \cdot y_{\mathrm{FSD}_{r,d}} \quad \forall r \in \mathrm{SU}, \forall d \in \mathrm{DU}\,. \tag{25}$$

Mixer treatment units

The mixer treatment unit MTU_t consists of a set of inlet streams from the splitter source unit, the initial splitter, the splitter process unit, and the splitter treatment unit.

The overall material balance for the mixer that is placed in front of the treatment unit is given by Eq. 26 and the mass balance for each contaminant j by Eq. 27:

$$\begin{aligned} \mathrm{FTU}_t^{\mathrm{in}} = \sum_{r\in \mathrm{SU}} \mathrm{FST}_{r,t} + \sum_{s\in \mathrm{SW}} \mathrm{FIT}_{s,t} + \sum_{p\in \mathrm{PU}} \mathrm{FPT}_{p,t} \\ + \sum_{\substack{t'\in \mathrm{TU} \\ t\ne t', R_t=0}} \mathrm{FT}_{t',t} + \sum_{\substack{t'\in \mathrm{TU} \\ R_t=1}} \mathrm{FT}_{t',t} \qquad \forall t \in \mathrm{TU} \end{aligned} \tag{26}$$

$$\begin{aligned} \mathrm{FTU}_t^{\mathrm{in}} \cdot x\mathrm{TU}_{t,j}^{\mathrm{in}} = \sum_{r\in \mathrm{SU}} \mathrm{FST}_{r,t} \cdot x\mathrm{SU}_{r,j}^{\mathrm{out}} + \sum_{s\in \mathrm{SW}} \mathrm{FIT}_{s,t} \cdot xW_{s,j}^{W} \\ + \sum_{p\in \mathrm{PU}} \mathrm{FPT}_{p,t} \cdot x\mathrm{SPU}_{p,j}^{\mathrm{out}} + \sum_{\substack{t'\in \mathrm{TU} \\ t\ne t', R_{TU}=0}} FT_{t',t} \cdot x\mathrm{STU}_{t,j}^{\mathrm{out}} \\ + \sum_{\substack{t'\in \mathrm{TU} \\ R_{\mathrm{TU}}=1}} \mathrm{FT}_{t',t} \cdot x\mathrm{STU}_{t,j}^{\mathrm{out}} \qquad \forall t \in \mathrm{TU}, \forall j. \end{aligned} \tag{27}$$

Treatment units

The treatment unit TU_t consists of an inlet stream from the mixer treatment unit, and an outlet stream from the treatment unit. The inlet and outlet flows for a treatment unit are equal and the overall material balance is given by Eq. 28.

$$\mathrm{FTU}_t^{\mathrm{in}} = \mathrm{FTU}_t^{\mathrm{out}} \quad \forall t \in \mathrm{TU}\,. \tag{28}$$

The mass balance equation for each contaminant j for the treatment unit $t \in \mathrm{TU}$ is assumed to be a linear function in terms of the recovery RR_{tj} given by Eq. 29.

$$x\mathrm{TU}_{t,j}^{\mathrm{out}} = \beta_{\mathrm{TU}_{t,j}} \cdot x\mathrm{TU}_{t,j}^{\mathrm{in}} \quad \forall t \in \mathrm{TU}, \forall j \tag{29}$$

where $\beta_{\mathrm{TU}t,j} = (1-\mathrm{RR}_{t,j}/100)$ for $\forall t \in \mathrm{TU}$, $\forall j$.

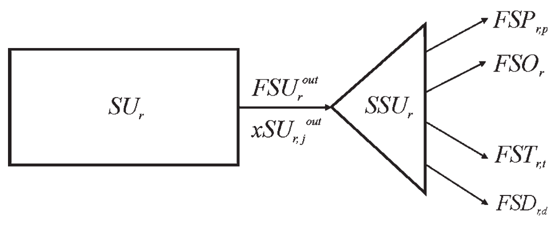

Figure 3. Source process unit.

Splitter treatment units

The splitter treatment unit STU_t consists of an inlet stream from the treatment unit and a set of outlet streams directed to the mixer demand unit, the mixer process unit, the final mixer, and the mixer treatment unit.

The overall material balance for the splitter process unit is given by equation (Eq. 30) and the equality of concentrations of the treatment unit and the splitter treatment unit by Eq. 31:

$$\mathrm{FTU}_t^{\mathrm{out}} = \sum_{d\in \mathrm{DU}} \mathrm{FTD}_{t,d} + \sum_{p\in \mathrm{PU}} \mathrm{FTP}_{t,p} + \mathrm{FTO}_t + \sum_{\substack{t'\in \mathrm{TU}\\ t\neq t', R_t=0}} \mathrm{FT}_{t',t} + \sum_{\substack{t'\in \mathrm{TU}\\ R_t=1}} \mathrm{FT}_{t',t} \qquad \forall t\in \mathrm{TU} \tag{30}$$

$$x\mathrm{STU}_{t,j}^{\mathrm{out}} = x\mathrm{TU}_{t,j}^{\mathrm{out}} \quad \forall t\in \mathrm{TU}, \forall j. \tag{31}$$

The lower and upper bound constraints that relate the flows and 0–1 variables for streams between the splitter treatment units and all mixers in the network are given as follows.

$$\mathrm{FTD}_{t,d}^{\mathrm{L}}\cdot y_{\mathrm{FTD}_{t,d}} \le \mathrm{FTD}_{t,d} \le \mathrm{FTD}_{t,d}^{\mathrm{U}}\cdot y_{\mathrm{FTD}_{t,d}} \quad \forall t\in TU, \forall d\in \mathrm{DU} \tag{32}$$

$$\mathrm{FTP}_{t,p}^{\mathrm{L}}\cdot y_{\mathrm{FTP}_{t,p}} \le \mathrm{FTP}_{t,p} \le \mathrm{FTP}_{t,p}^{\mathrm{U}}\cdot y_{\mathrm{FTP}_{t,p}} \quad \forall t\in \mathrm{TU}, \forall p\in \mathrm{PU} \tag{33}$$

$$\mathrm{FTO}_t^{\mathrm{L}}\cdot y_{\mathrm{FTO}_t} \le \mathrm{FTO}_t \le \mathrm{FTO}_t^{\mathrm{U}}\cdot y_{\mathrm{FTO}_t} \quad \forall t\in \mathrm{TU} \tag{34}$$

$$\mathrm{FT}_{t',t}^{\mathrm{L}}\cdot y_{\mathrm{FT}_{t',t}} \le \mathrm{FT}_{t',t} \le \mathrm{FT}_{t',t}^{\mathrm{U}}\cdot y_{\mathrm{FT}_{t',t}} \quad \forall t\in \mathrm{TU}, \forall t'\in \mathrm{TU}, t'\neq t, R_t=0 \tag{35}$$

$$\mathrm{FT}_{t',t}^{\mathrm{L}}\cdot y_{\mathrm{FT}_{t',t}} \le \mathrm{FT}_{t',t} \le \mathrm{FT}_{t',t}^{\mathrm{U}}\cdot y_{\mathrm{FT}_{t',t}} \quad \forall t\in \mathrm{TU}, \forall t'\in \mathrm{TU}, R_t=1. \tag{36}$$

Final mixer

The final mixer unit MF consists of a set of inlet streams from the initial splitter, the splitter process unit, the splitter treatment unit, and the splitter source unit.

The overall material balance for the final mixer is given by Eq. 37 and the mass balance equation for each contaminant j by Eq. 38:

$$F^{\mathrm{out}} = \sum_{s\in \mathrm{SW}} \mathrm{FIF}_s + \sum_{p\in \mathrm{PU}} \mathrm{FPO}_p + \sum_{t\in \mathrm{TU}} \mathrm{FTO}_t + \sum_{r\in \mathrm{SU}} \mathrm{FSO}_r \tag{37}$$

$$F^{\mathrm{out}}\cdot x_j^{\mathrm{out}} = \sum_{s\in \mathrm{SW}} \mathrm{FIF}_s\cdot xW_{s,j}^{\mathrm{in}} + \sum_{p\in PU} \mathrm{FPO}_p\cdot x\mathrm{SPU}_{p,j}^{\mathrm{out}} + \sum_{t\in \mathrm{TU}} \mathrm{FTO}_t\cdot x\mathrm{STU}_{t,j}^{\mathrm{out}} + \sum_{r\in \mathrm{SU}} \mathrm{FSO}_r\cdot x\mathrm{SU}_{r,j}^{\mathrm{out}} \qquad \forall j. \tag{38}$$

Using the binary variables for the existence of pipe connections, the specification for a maximum number of these connections in the network is given by Eq. 39. Using this constraint for different values of $N_{\max}$ it is possible to establish optimal trade-offs between network cost and network complexity.

$$\begin{aligned}
&\sum_{s\in \mathrm{SW}}\sum_{p\in \mathrm{PU}} y_{\mathrm{FIP}_{s,p}} + \sum_{s\in \mathrm{SW}}\sum_{t\in \mathrm{TU}} y_{\mathrm{FIT}_{s,t}} + \sum_{s\in \mathrm{SW}} y_{\mathrm{FIF}_s} \\
&+ \sum_{\substack{p'\in \mathrm{PU}\\ p'\neq p, R_p=0}}\sum_{p\in \mathrm{PU}} y_{\mathrm{FP}_{p',p}} + \sum_{\substack{p'\in \mathrm{PU}\\ R_{\mathrm{PU}}=1}}\sum_{p\in \mathrm{PU}} y_{\mathrm{FP}_{p',p}} + \sum_{p\in \mathrm{PU}} y_{\mathrm{FPO}_p} \\
&+ \sum_{p\in \mathrm{PU}}\sum_{t\in \mathrm{TU}} y_{\mathrm{FPT}_{p,t}} + \sum_{\substack{t'\in \mathrm{TU}\\ t'\neq t, R_t=0}}\sum_{t\in \mathrm{TU}} y_{\mathrm{FT}_{t',t}} + \sum_{\substack{t'\in \mathrm{TU}\\ R_t=1}}\sum_{t\in \mathrm{TU}} y_{\mathrm{FT}_{t',t}} \\
&+ \sum_{t\in \mathrm{TU}} y_{\mathrm{FTO}_t} + \sum_{t\in \mathrm{TU}}\sum_{p\in \mathrm{PU}} y_{\mathrm{FTP}_{t,p}} + \sum_{s\in \mathrm{SW}}\sum_{d\in \mathrm{DU}} y_{\mathrm{FID}_{s,d}} \\
&+ \sum_{p\in \mathrm{PU}}\sum_{d\in \mathrm{DU}} y_{\mathrm{FPD}_{p,d}} + \sum_{t\in \mathrm{TU}}\sum_{d\in \mathrm{DU}} y_{\mathrm{FTD}_{t,d}} + \sum_{r\in \mathrm{SU}}\sum_{d\in \mathrm{DU}} y_{\mathrm{FSD}_{r,d}} \\
&+ \sum_{r\in \mathrm{SU}} y_{\mathrm{FSO}_r} + \sum_{r\in \mathrm{SU}}\sum_{t\in \mathrm{TU}} y_{\mathrm{FST}_{r,t}} + \sum_{r\in \mathrm{SU}}\sum_{p\in \mathrm{PU}} y_{\mathrm{FSP}_{r,p}} \le N_{\max}
\end{aligned} \tag{39}$$

Objective function of the NLP and MINLP model

The MINLP model in the previous section reduces to an NLP in the case that binary variables with their corresponding lower and upper bound constraints (2–5, 13–17, 22–25, 32–36, 39) are excluded from the model. The objective function of the NLP water network problems can simply be formulated to minimize the total consumption of freshwater for network plant operation and the total amount of wastewater treated in treatment operations for an integrated system.[1]

$$\min Z = \sum_{s\in \mathrm{SW}} \mathrm{FW}_s + \sum_{t\in \mathrm{TU}} \mathrm{FTU}_t^{\mathrm{out}}. \tag{40}$$

For separate subsystems consisting of water-using or wastewater treatment operations the objective function is to either minimize the total consumption of freshwater or the total amount of wastewater treated in treatment operations, respectively.

$$\min Z = \sum_{s\in \mathrm{SW}} \mathrm{FW}_s \tag{41}$$

$$\min Z = \sum_{t\in \mathrm{TU}} \mathrm{FTU}_t^{\mathrm{out}}. \tag{42}$$

A more accurate objective function for the NLP model is to minimize the total network cost consisting of the cost of freshwater, the cost of investment on treatment units, and the operating cost for the treatment units. This type of objective function is used in many articles to optimize the water network problems.

$$\min Z = H\cdot \sum_{s\in \mathrm{SW}} \mathrm{FW}_s\cdot \mathrm{CFW}_s + \mathrm{AR}\cdot \sum_{t\in \mathrm{TU}} \mathrm{IC}_t\cdot \left(\mathrm{FTU}_t^{\mathrm{out}}\right)^{\alpha} + H\cdot \sum_{t\in \mathrm{TU}} \mathrm{OC}_t\cdot \mathrm{FTU}_t^{\mathrm{out}}. \tag{43}$$

Furthermore, in the case of separate subsystems consisting of water-using or wastewater treatment operations the objective function is to minimize the total cost of water, or the total cost of investment on treatment units and operating cost for the treatment units:

$$\min Z = H \cdot \sum_{s\in SW} FW_s \cdot CFW_s \tag{44}$$

$$\min Z = AR \cdot \sum_{t\in TU} IC_t \cdot \left(FTU_t^{out}\right)^{\alpha} + H \cdot \sum_{t\in TU} OC_t \cdot FTU_t^{out}. \tag{45}$$

The objective function for the MINLP model is to minimize the total network cost given by Eq. 46, which includes the cost of the network piping (concave function of the flowrate with fixed charge) and the cost of water pumping through pipes (linear function of the flowrate):

$$\min Z = C_{water} + IC_{treatment} + OC_{treatment} + OC_{water\,pumping} + IC_{pipes}. \tag{46}$$

Here, C_{water} is the yearly cost of water for the network plant operation; $IC_{treatment}$ is the investment cost for treatment units; $OC_{treatment}$ is the yearly operating cost for treatment units; $OC_{pumping}$ is the yearly operating cost for pumping water through pipes in the network under the assumption that the pressure drop in each pipe section is fixed (or equivalently that the flow velocity is fixed[34]); IC_{pipes} is the investment cost of the pipes in the network. The annualized costs are expressed for each term in Eq. 46 as follows.

$$C_{water} = H \cdot \sum_{s\in SW} FW_s \cdot CFW_s \tag{46a}$$

$$IC_{treatment} = AR \cdot \sum_{t\in TU} IC_t \cdot \left(FTU_t^{out}\right)^{\alpha} \tag{46b}$$

$$OC_{treatment} = H \cdot \sum_{t\in TU} OC_t \cdot FTU_t^{out} \tag{46c}$$

$$\begin{aligned} OC_{pumping} = H \cdot \Bigg[& \sum_{s\in SW}\sum_{p\in PU} FIP_{s,p} \cdot PM_p + \sum_{s\in SW}\sum_{t\in TU} FIT_{s,t} \cdot PM_t + \sum_{t\in TU}\sum_{p\in PU} FTP_{t,p} \cdot PM_t + \sum_{\substack{p'\in PU\\ R_p=1}}\sum_{p\in PU} FP_{p',p} \cdot PM_{p'} \\ & + \sum_{\substack{p'\in PU\\ p'\neq p, R_p=0}}\sum_{p\in PU} FP_{p',p} \cdot PM_{p'} + \sum_{p\in PU}\sum_{t\in TU} FPT_{p,t} \cdot PM_p + \sum_{p\in PU} FPO_p \cdot PM_p + \sum_{t\in TU} FTO_t \cdot PM_t + \sum_{\substack{t'\in TU\\ R_t=1}}\sum_{t\in TU} FT_{t',t} \cdot PM_{t'} \\ & + \sum_{\substack{t'\in TU\\ t'\neq t, R_{TU}=0}}\sum_{t\in TU} FT_{t',t} \cdot PM_{t'} + \sum_{s\in SW}\sum_{d\in DU} FID_{s,d} \cdot PM_d + \sum_{p\in PU}\sum_{d\in DU} FPD_{p,d} \cdot PM_d + \sum_{t\in TU}\sum_{d\in DU} FTD_{t,d} \cdot PM_d \\ & + \sum_{r\in SU}\sum_{d\in DU} FSD_{r,d} \cdot PM_d + \sum_{r\in SU}\sum_{p\in PU} FSP_{r,p} \cdot PM_p + \sum_{r\in SU}\sum_{t\in TU} FST_{r,t} \cdot PM_t + \sum_{r\in SU} FSO_r \cdot PM_r \Bigg] \end{aligned} \tag{46d}$$

$$\begin{aligned} IC_{pipes} = AR \cdot \Bigg[& \sum_{t\in TU}\sum_{p\in PU} (CP_t \cdot y_{FTP_{t,p}} + IP_t \cdot (FTP_{t,p}))^{\gamma} + \sum_{\substack{p'\in PU\\ R_p=1}}\sum_{p\in PU} (CP_{p'} \cdot y_{FP_{p',p}} + IP_{p'} \cdot (FP_{p',p})^{\gamma}) \\ & + \sum_{\substack{p'\in PU\\ p'\neq p, R_p=0}}\sum_{p\in PU} (CP_{p'} \cdot y_{FP_{p',p}} + IP_{p'} \cdot (FP_{p',p})^{\gamma}) + \sum_{p\in PU}\sum_{t\in TU} (CP_p \cdot y_{FPT_{p,t}} + IP_p \cdot (FPT_{p,t})^{\gamma}) \\ & + \sum_{p\in PU} (CP_p \cdot y_{FPO_p} + IP_p \cdot (FPO_p)^{\gamma}) + \sum_{t\in TU} (CP_t \cdot y_{FTO_t} + IP_t \cdot (FTO_t)^{\gamma}) \\ & + \sum_{\substack{t'\in TU\\ R_t=1}}\sum_{t\in TU} (CP_{t'} \cdot y_{FT_{t',t}} + IP_{t'} \cdot (FT_{t',t})^{\gamma}) + \sum_{\substack{t'\in TU\\ t'\neq t, R_{TU}=0}}\sum_{t\in TU} (CP_{t'} \cdot y_{FT_{t',t}} + IP_{t'} \cdot (FT_{t',t})^{\gamma}) \\ & + \sum_{s\in SW}\sum_{p\in PU} (CP_p \cdot y_{FIP_{s,p}} + IP_p \cdot (FIP_{s,p})^{\gamma}) + \sum_{s\in SW}\sum_{t\in TU} (CP_t \cdot y_{FIT_{s,t}} + IP_t \cdot (FIT_{s,t})^{\gamma}) \\ & + \sum_{s\in SW}\sum_{d\in DU} (CP_d \cdot y_{FID_{s,d}} + IP_d \cdot (FID_{s,d})^{\gamma}) + \sum_{p\in PU}\sum_{d\in DU} (CP_d \cdot y_{FPD_{p,d}} + IP_d \cdot (FP_{s,d})^{\gamma}) \\ & + \sum_{t\in TU}\sum_{d\in DU} (CP_d \cdot y_{FTD_{t,d}} + IP_d \cdot (FTD_{t,d})^{\gamma}) + \sum_{r\in SU}\sum_{d\in DU} (CP_d \cdot y_{FSD_{r,d}} + IP_d \cdot (FSD_{r,d})^{\gamma}) \\ & + \sum_{r\in SU} (CP_r \cdot y_{FSO_r} + IP_r \cdot (FSO_r)^{\gamma}) + \sum_{r\in SU}\sum_{t\in TU} (CP_t \cdot y_{FST_{r,t}} + IP_t \cdot (FST_{r,t})^{\gamma}) \\ & + \sum_{r\in SU}\sum_{p\in PU} (CP_p \cdot y_{FSP_{r,p}} + IP_p \cdot (FSP_{r,p})^{\gamma} \Bigg]. \end{aligned} \tag{46e}$$

Notice that concave cost functions are involved in Eqs. 46b and 46e, which are additional sources of nonconvexities to the bilinearities in the mixer Eqs. 7, 19, 27, and 38.

Solution Strategy

The proposed model presented in the previous section corresponds to a nonconvex NLP or nonconvex MINLP problem. This problem is modeled in GAMS.[42] In this article, BARON[41] is used for solving all water network problems to rigorous global optimality.

To effectively solve the NLP and MINLP problems to global optimality it is important to be able to obtain tight lower bounds on the global optimum. To significantly improve the strength of this lower bound we incorporate the cut proposed by Karuppiah and Grossmann.[1] These authors found that by adding this redundant constraint to the model instead of using their specialized algorithm, they could solve their NLP model to global optimality directly with BARON in orders of magnitude less time. The bound strengthening in the nonlinear model corresponds to the contaminant flow balances for the overall water network system and is given by equation:

$$\sum_{s\in \mathrm{SW}} \mathrm{FW}_s \cdot xW^{\mathrm{in}}_{s,j} + \sum_{p\in \mathrm{PU}} \mathrm{LPU}_{p,j} + \sum_{r\in \mathrm{SU}} \mathrm{FSU}^{\mathrm{out}}_r \cdot x\mathrm{SU}^{\mathrm{out}}_{r,j} = \sum_{t\in \mathrm{TU}} (1-\beta_{\mathrm{TU}_{t,j}}) \cdot \mathrm{FTU}^{\mathrm{in}}_t \cdot x\mathrm{TU}^{\mathrm{in}}_{t,j} + F^{\mathrm{out}} \cdot x^{\mathrm{out}}_j + \sum_{d\in \mathrm{DU}} \mathrm{FDU}^{\mathrm{in}}_d \cdot x\mathrm{DU}^{\mathrm{in}}_{d,j} \quad \forall j \tag{47}$$

where bilinear terms are involved for the treatment units and final mixing points. Qualitatively, the reason for the effectiveness of his cut is that it imposes the overall mass balance for each contaminant given that the mass balances are relaxed at the mixing nodes with the McCormick convex envelopes that are used to replace the bilinear terms in 7, 19, 27, and 38.

It is also worth pointing out that when solving nonconvex water network problems by the previously mentioned global optimization solvers, it is important to specify tight variable bounds for all flowrates and concentrations in the water network. The reason is that these bounds are used in the convex envelopes for under and overestimating the nonconvexities (e.g., secant for concave function or McCormick envelopes for bilinear terms). In the proposed model, the bounds on the variables are represented as general equations as shown in the Appendix. They are obtained by physical inspection of the superstructure and by using logic specifications. Using the proposed model with the cuts by Karuppiah and Grossmann[1] and the bounds in the Appendix we can effectively solve the NLP water network problems for different levels of complexity with multiple sources of water, multiple contaminants, and more process and treatment units (large-scale problems). Also, the MINLP water network problems can be effectively solved to rigorous global optimality using the proposed model.

As for the implementation of the proposed models, it is important to note that the derivatives become unbounded when the flows take zero values in the cost terms given by Eqs. 46b and 46e (investment costs of pipes and treatment units). To circumvent this problem, we add a tolerance ε (typically 0.001) in the cost function [Cost $= a\cdot(\mathrm{Flow}+\varepsilon)^b$] for the investment cost of the pipes in the network and for treatment units. Although this introduces a small error in the cost function (e.g., about 0.001% for example 5 with $\varepsilon = 0.001$), it leads to bounded gradients for zero flows.

We also propose a two-stage solution strategy that can be used for solving more quickly large-scale MINLP industrial water network problems. First, we solve the relaxed MINLP to global optimality which yields a valid lower bound (LB). We then fix all zero flowrates in the network and update the variable bounds before solving the reduced MINLP, also to global optimality, which yields an upper bound (UB). The optimality gap of the solution of the reduced MINLP can then simply be calculated as follows: optimality gap = (UB−LB)/UB, which gives a measure of the maximum deviation of the solution obtained by the reduced MINLP with respect to the global optimum. Although global optimality cannot be guaranteed with this two stage procedure, in our experience the rigorous global solution is obtained in most cases. Furthermore, the optimality gap is usually very small.

In the case when we want to establish optimal trade-offs between cost and network complexity, we solve the MINLP by successively reducing the maximum number of pipe segments to obtain the Pareto-optimal curve. More specifically, after solving the original MINLP model we solve it by successively reducing the number of piping connections. It that case, we specify the maximum number of piping connections to be $N^{\mathrm{MINLP}}_{\mathrm{streams}} - N$, where N is the number of piping connections to be reduced for simplifying the network.

Examples

In this section, we present six examples to illustrate the proposed optimization models. All examples were implemented in GAMS[42] and solved on a HP Pavilion Notebook PC with 4 GB RAM memory, and Intel Core Duo 2 GHz processor. The general purpose global optimization solver BARON[41] is used for solving the examples to global optimality. Model statistics, problems sizes, and computational times are reported at the end of the six example problems.

Example 1

In this example, we illustrate the advantage of using local recycles around the process units in the network. Moreover, it is shown how to establish optimal trade-offs between costs and complexity of the water networks in terms of number of piping connections. The water network superstructure for this example is shown in Figure 4. It consists of two process, two treatment units and a single source of water.

Data of process units, treatment units, and contaminants are given in Tables 1 and 2, respectively, and are taken from Karuppiah and Grossmann.[1]

Each treatment unit can remove only one contaminant. The environmental discharge limit for contaminant A and contaminant B is 10 ppm. The freshwater cost is assumed to be $1/ton, the annualized factor for investment is taken to be 0.1, and the total time for the network plant operation in a year is assumed to be 8000 h. We formulated the problem as

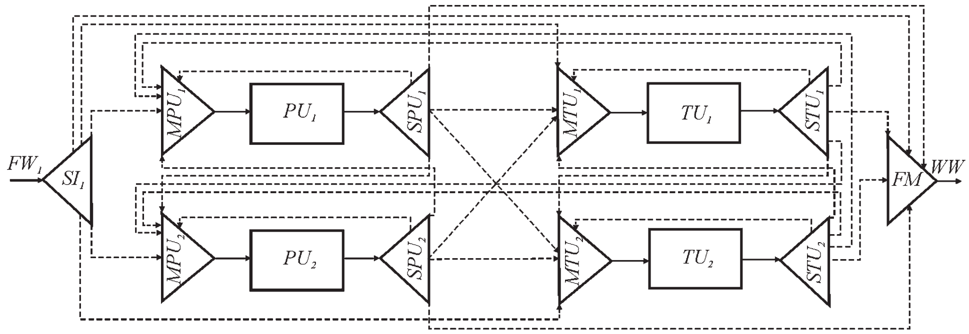

Figure 4. Water network superstructure for Example 1.

Table 1. Data for Process Units (Example 1)

Unit	Flowrate (t/h)	Discharge Load (kg/h)		Maximum Inlet Concentration (ppm)	
		A	*B*	*A*	*B*
PU_1	40	1	1.5	0	0
PU_2	50	1	1	50	50

the nonconvex NLP where the objective function is to minimize the total network cost given by Eq. 43. The optimal tolerance selected for the optimization with BARON was zero. The global optimization results are given in Table 3.

With the local recycle around the process unit it is possible to meet both flowrate and contaminant constraints at the process unit inlets and have lower total network cost ($584016.9/year) compared to the case without local recycle ($596163.6/year) (see Figure 5). Note that the reduction is due to savings in the treatment units.

In addition to this, we directly solved the same example as the MINLP for the case when the investment cost for piping and the operating cost for pumping water inside pipes are included in the objective function (see Eq. 46). In this example, the fixed cost pertaining to the pipes is assumed to be $6, the variable cost for each individual pipe $100, and operating cost coefficient for pumping water through pipes $0.006/ton as given by Karuppiah and Grossmann.[39] The global optimization results are given in Table 4. It should be noted, that both the NLP and MINLP problem for each case (with or without local recycles) have the same optimal design of water network as shown in Figures 5 and 6. As can be seen from Figures 5 and 6 the number of ''removable'' piping connections (i.e., streams between all splitters and mixers in that may not exist in the final solution) for the NLP and MINLP problem without local recycle is 8 and with local recycle it is 9. In addition, removable connections are shown in Figure 4 as dashed lines that may be actually deleted from the superstructure. According to this, it is useful for the designer to have a tool which can be used to establish optimal trade-offs between the network cost and network complexity. This can be accomplished by adding constraint 39 to the MINLP by specifying a maximum number of allowable connections from the set of removable streams. For the water networks given in Figures 5 and 6, and the same data for the MINLP problem, the results of the Pareto-optimal solutions are shown in Table 5.

The optimal network cost for the option without local recycle is $606760.55/year, and with local recycle $593991.11/year. In the first case, the number of removable connections is 8 and in the second it is 9. To simplify the network we added constraint Eq. 39. Figure 7 shows the results of the water network optimization for different number of removable streams. For instance, we can greatly simplify the water network with six removable piping connections as shown in Figures 8 and 9, while we still keep the freshwater consumption at 40 t/h although the cost increases by 17% due to the larger flows in the treatment units.

As can be seen from Table 5 the total network cost for the option without local recycle is somewhat higher compared to the case with local recycle. The main reason is the higher wastewater flowrate (50 t/h) which must be treated in treatment unit TU_2.

To illustrate the capability of the proposed model to solve the class of water network problems with variable flowrates through water-using process units, we solved the corresponding MINLP problem from this example. In this case, the flowrate is a continuous variable to be determined by the optimization. In addition, for this problem, the maximum inlet and outlet contaminant concentration, and mass load of contaminant at the water-using process units must be specified (see Table 6). On the basis of the data given in Table 6 the limiting water flowrate can be determined and used for

Table 2. Data for Treatment Units (Example 1)

Unit	Percentage Removal of Contaminant		IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
	A	*B*			
TU_1	95	0	16,800	1	0.7
TU_2	0	95	12,600	0.0067	0.7

Table 3. Optimization Results for the NLP Water Network Problem (Example 1)

	Without Recycle	With Recycle
Freshwater cost	$320000	$320000
Investment cost of treatment units	$37440	$33585.3
Operating costs of treatment units	$238723.6	$230431.6
Total cost	$596163.6	$584016.9
Total time (s)	0.37	1

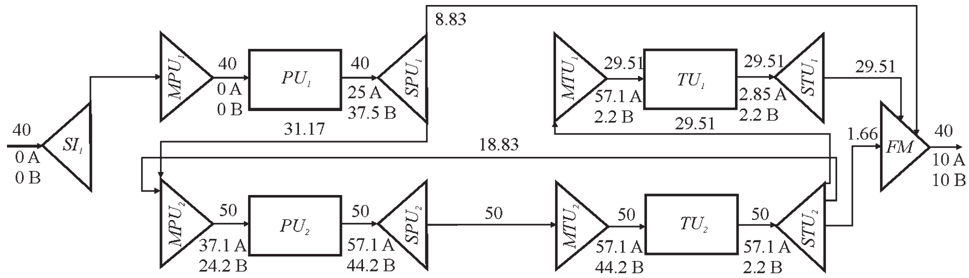

Figure 5. Optimal solution for the NLP and MINLP problem without local recycle (Example 1).

Table 4. Optimization Results for the MINLP Water Network Problem (Example 1)

	Without Recycle	With Recycle
Freshwater cost	\$320000	\$320000
Investment cost on pipes	\$540.69	\$546.3
Operating cost for pumping water	\$10056.26	\$9427.84
Investment cost of treatment units	\$37440.01	\$33585.32
Operating costs of treatment units	\$238723.59	\$230431.64
Total cost	\$606760.55	\$593991.1
Total time (s)	3.6	2.5

calculation of the variable bounds as given in the Appendix. All other data for this problem are the same as data given for the MINLP problem with fixed flowrate through the water-using process units. The optimal tolerance selected for the optimization with BARON was zero. The optimum solution (\$592897.99/year) of water network with eight removable connections is obtained in 13.2 CPUs. The freshwater consumption (40 t/h) was the same as the obtained solution for the flowrate fixed. However, the total network cost and the flowrate through the process unit 2 (\$592897.99/year, 28.55 t/h) were smaller than in the case of the fixed flowrate (\$596012.94/year, 50 t/h) for the network with eight removable streams.

Example 2

The main goal of this example is to demonstrate the capability of the proposed model to solve water network problems of different complexity to global optimality and to compare results with the ones reported in the literature. Data for this example is taken from the literature (Example 1–4 given by Karuppiah and Grossmann[1]). The relative optimality tolerance in all examples was set to 0.01. Here, we used the general purpose optimization software BARON to solve all the problems. The optimization results reported in the article given by Karuppiah and Grossmann[1] and the results obtained with the proposed model in this article are shown in Table 7.

The first problem involves a water network with two process units (PU) and two treatment (TU) units. The objective function was to minimize the total sum of the freshwater consumption and total flowrate of wastewater treated inside of treatment units (Eq. 40). Karuppiah and Grossmann[1] reported the optimal solution 117.05 t/h. However, they did not consider local recycle around the process unit which leads to a 13% reduction in the objective function as seen in Table 7.

In addition, as can be also seen in Table 7, we solved water network problems with three process and three treatment units, four process and two treatment units, five process and three treatment units. For these examples, the values of the objective function (minimum total network cost) obtained by the proposed model in this article are the same as the ones reported by Karuppiah and Grossmann,[1] while the computational time is smaller in all cases. The main reasons for improved performance are good variable bounds for all flowrates and concentrations, incorporating the cut proposed by Karuppiah and Grossmann[1] and a faster computer.

Example 3

This example demonstrates the capability of the proposed model to solve water network problems with both mass transfer and non-mass transfer operations. The case study, a Specialty Chemical Plant, is taken from Wang and Smith.[15] The process flowsheet is given in Figure 10, which has a consumption of 165 t/h freshwater. It should be noted that the water entering the process is greater than the wastewater flow in the exit since some water leaves the process with the product. Table 8 gives limiting process data for water-using operations in the process and its utility system.

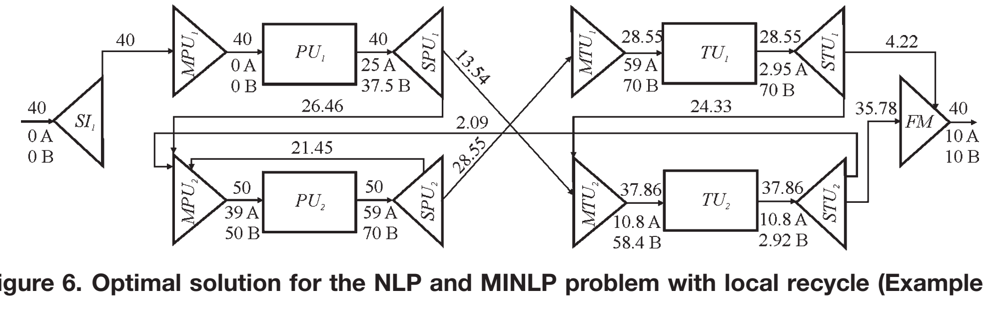

Figure 6. Optimal solution for the NLP and MINLP problem with local recycle (Example 1).

Table 5. Results of Establishing the Trade-Off Between the Network Cost and Network Complexity

Total Cost ($/year)		Number of Removable Streams in the Network	
Without Local Recycle	With Local Recycle	Without Local Recycle	With Local Recycle
–	593991.11	–	9
606760.55	596012.94	8	8
620857.57	613610.77	7	7
695456.90	691610.36	6	6

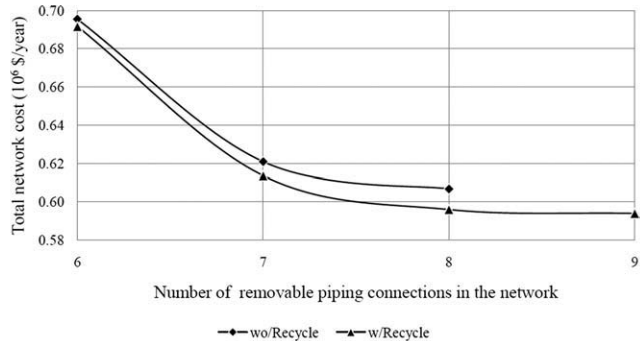

Figure 7. Pareto-optimal solutions for minimum cost and minimum number of removable connections for Example 1.

Water-using operations such as the reactor, filtration, and cooling tower have different water flowrates at their inlets and outlets. In the case of the reactor and the cooling tower there are losses of water. However, in the case of filtration process there is gain of water. Water flowrates of these operations can be divided in two parts. The first part is considered to be unchanged through the process, while the second part involves loss or gain of water.[15] According to this, the modified process data for this example are given in Table 9.

According to the flowsheet in Figure 10, the operations that can be considered as the water sink/demand units are reactor and cooling tower. The water source unit is filtration. Representation of these units and their flowrates is shown in Figures 11 and 12, respectively.

The global optimal solution of the NLP model for the water network with reuse for the data in Table 9 is given in Figure 13. The optimization was performed with the global optimization BARON solver and the selected optimality tolerance was zero. The objective function was to minimize the total consumption of freshwater for network. The new water network design yields reductions in freshwater consumption of about 45% (from 165 t/h to 90.64 t/h) and wastewater generation of about 59% (from 125 t/h to 50.64 t/h). It is worth to mention that the values of water consumption and wastewater generation are the same as the ones reported by Wang and Smith[15] and Bandyopadhyay et al.[23]

In addition to this, Bandyopadhyay et al.[23] solved the same problem using their proposed method for targeting minimum effluent treatment flowrate satisfying the minimum freshwater requirement. In their article the water allocation network incorporates two treatment units. They assumed the percent removal of each contaminant in treatment units to be 90, and maximum allowable concentration of contaminants in the discharge effluent to the environment to be 50 ppm. We solved the same problem by sequential optimization of water-using and water treatment units. The objective function for optimization of water using operations is to minimize the sum of freshwater consumption and the objective function for optimization of treatment operations is to minimize the sum of water flowrates going to treatment units.

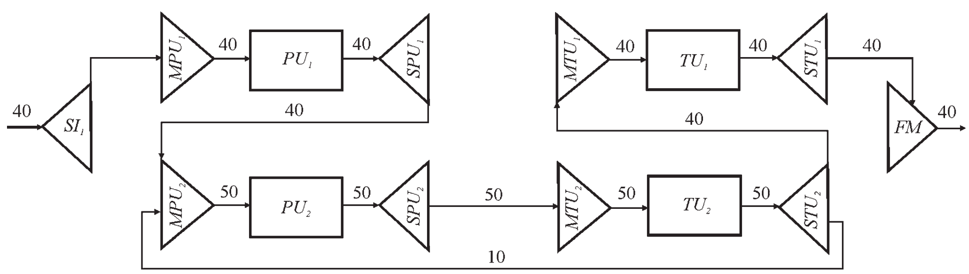

Figure 8. Water network with six removable streams and without local recycle (Example 1).

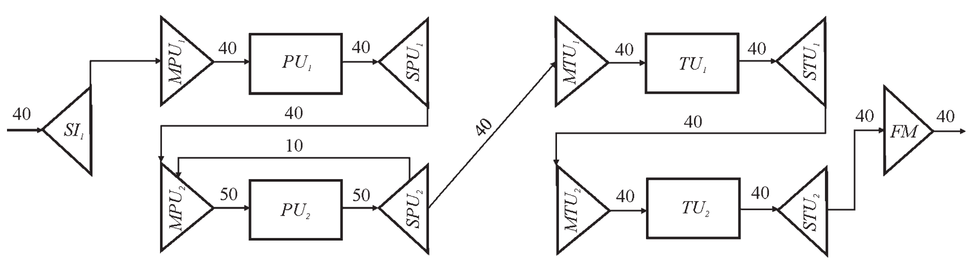

Figure 9. Water network with six removable streams and with local recycle (Example 1).

Table 6. Data for the Variable Flowrates Through the Process Units (Example 1)

	Discharge Load (kg/h)		Maximum Inlet Concentration (ppm)		Maximum Outlet Concentration (ppm)		
Unit	*A*	*B*	*A*	*B*	*A*	*B*	Limiting Water Flowrate (t/h)
PU_1	1	1.5	0	0	25	37.5	40
PU_2	1	1	50	50	70	70	50

Table 7. Comparison Optimization Results for NLP Problems Different Complexity (Example 2)

		Results given by Karuppiah and Grossmann[1]		Proposed NLP Method	
Problem	No Units	Global Optimum	Total Time (s)	Global Optimum	Total Time (s)
1	2PU-2TU	117.05 t/h	37.72	101.57 t/h	0.36
2	3PU-3TU	$381751.35	13.21	$381751.35	0.34
3	4PU-2TU	$874057.37	0.90	$874057.37	0.11
4	5PU-3TU	$1033810.95	231.37	$1033810.95	16.15

The optimal network design is the same as reported by Bandyopadhyay et al.[23] (freshwater consumption of 90.64 t/h). However, we also optimized simultaneously the same problem as an integrated network with the water-using operations and water treatment operations. We assumed to have two treatment units with the same percent removal of contaminant in the treatment units (90%). Also, we considered the options with/without local recycle around process units. In both cases, the new designs yield a reduction in freshwater consumption of about 73% (from 165 t/h to 45 t/h) and wastewater generation of about 96% (from 125 t/h to 5 t/h)

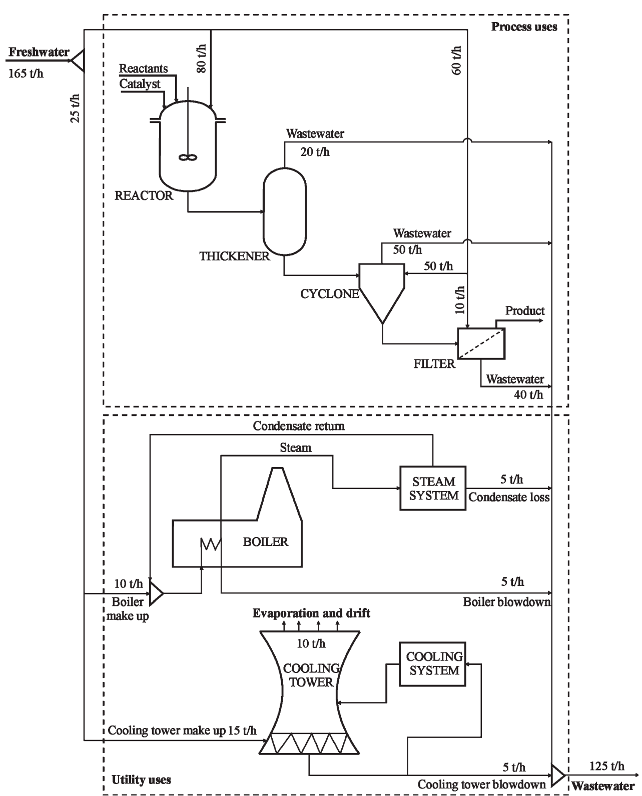

Figure 10. Flowsheet for specialty chemical plant with its utility systems.

compared to the base case. Moreover, we assumed to have two treatment units for wastewater treatment, but only one is selected by the optimization. The optimal solution of the water network design with recycle around process unit is given in Figure 14.

Example 4

In the process industry water-using operations can have different maximum allowed concentrations at their inlets. Therefore, water sources of different quality can be used to satisfy water-using concentration and flowrate demands. The higher quality water is more expensive than the lower quality water. The objective of this example is to illustrate that the proposed method can be applied to a complex industrial water network consisting of four sources of water, six water-using operations, three water treatment operations, and three contaminants. Data for water sources, water-using operations, and treatment units are given in Tables 10–12.

Data for the process and treatment units are taken from Karuppiah and Grossmann[1] and are slightly modified for this example. The annualized factor for investment of treatment units, the total time for the network plant operation, and maximum allowable contaminants concentration in the discharge effluent to the environment are the same as in Example 1 (0.1, 8000 h, 10 ppm). The objective function is to minimize the total network cost. The optimality tolerance selected for the global optimization of the NLP model was 0.05 with the global optimization solver BARON which required 2 CPUs (with 0.01 tolerance the time was about more than 5000 CPUs but yielded the same solution). The total cost for the network is $1149710.84/year, and the

Table 8. Limiting Process Data for Specialty Chemical Plant[15] (Example 3)

Operation	Water In (t/h)	Water Out (t/h)	c_{in} (ppm)	c_{out} (ppm)
Reactor	80	20	100	1000
Cyclone	50	50	200	700
Filtration	10	40	0	100
Steam system	10	10	0	10
Cooling system	15	5	10	100

Table 9. Modified Limiting Process Data for Specialty Chemical Plant (Example 3)

Operation	Water In (t/h)	Water Out (t/h)	c_{in} (ppm)	c_{out} (ppm)
Reactor I	20	20	100	1000
Reactor II	60	0	100	–
Cyclone	50	50	200	700
Filtration I	10	10	0	100
Filtration II	0	30	–	100
Steam system	10	10	0	10
Cooling system I	5	5	10	100
Cooling system II	10	0	10	–

optimal solution of the water network design is given in Figure 15. It should be noticed that the freshwater source 4 is not selected. In addition, pure water from source 1, which has the highest cost, is minimized at the expense of using more of the lower quality water.

Example 5

The objective of this example is to illustrate the application of the proposed MINLP solution method on a large-scale industrial network consisting of five water-using units, three wastewater treatment units, and three contaminants (A–C). Data for this example are given in Tables 13 and 14.[1]

The annualized factor for investment of the treatment units, the total time for the network plant operation, and maximum allowable contaminants concentration in the discharge effluent to the environment are the same as in Example 1 (0.1, 8000 h, 10 ppm). The objective function is to minimize the total network cost.

The MINLP model for this example is solved to global or near global optimality using the direct MINLP method as well as using the two-stage solution startegy. The optimality tolerance selected with BARON for optimization was 0.01. We added the tolerance $\varepsilon = 0.001$ in the cost function (Cost $= a \cdot (\text{Flow} + \varepsilon)^b$) for the investment cost of the pipes in the

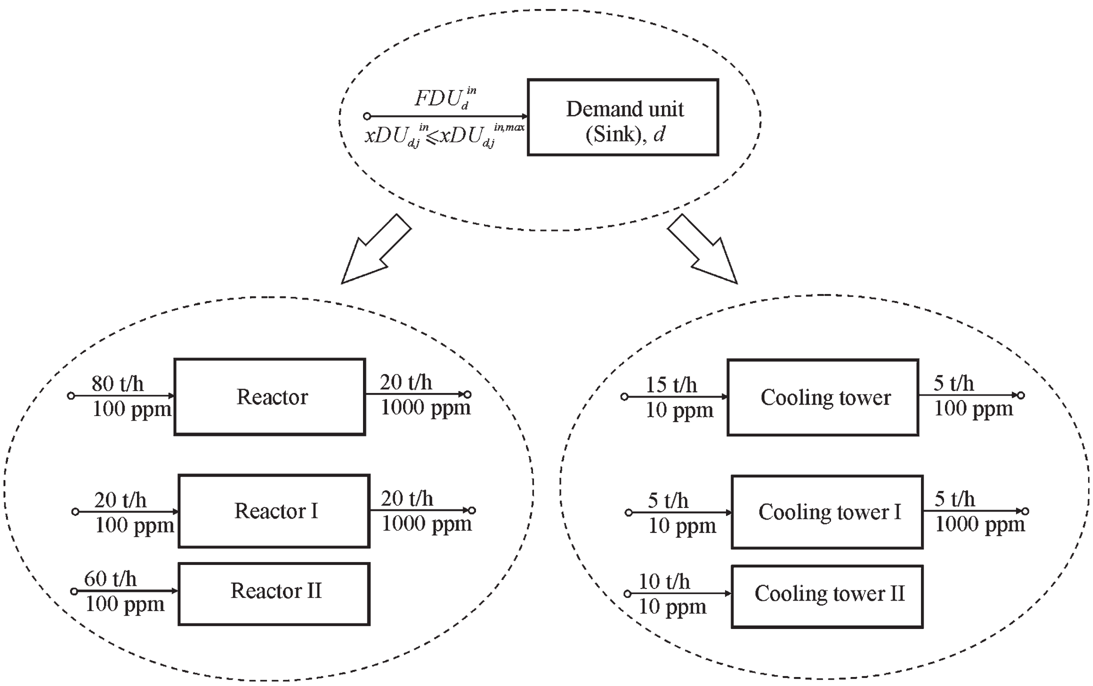

Figure 11. Representation of flowrates of the water demand unit.

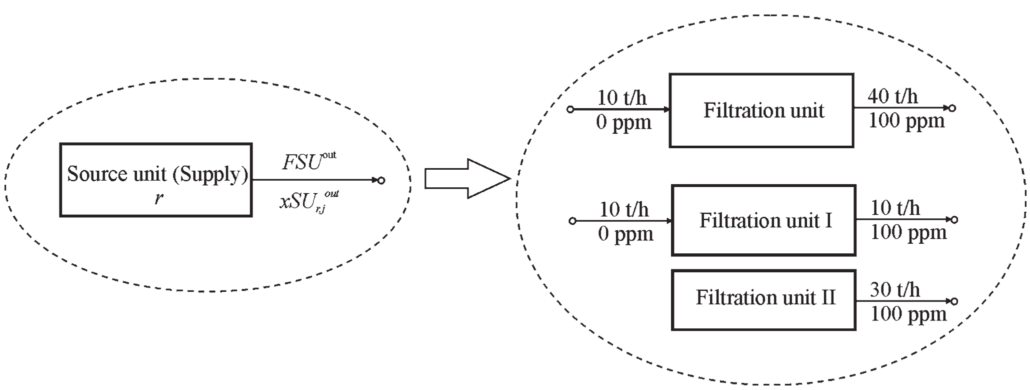

Figure 12. Representation of flowrates of the water source unit.

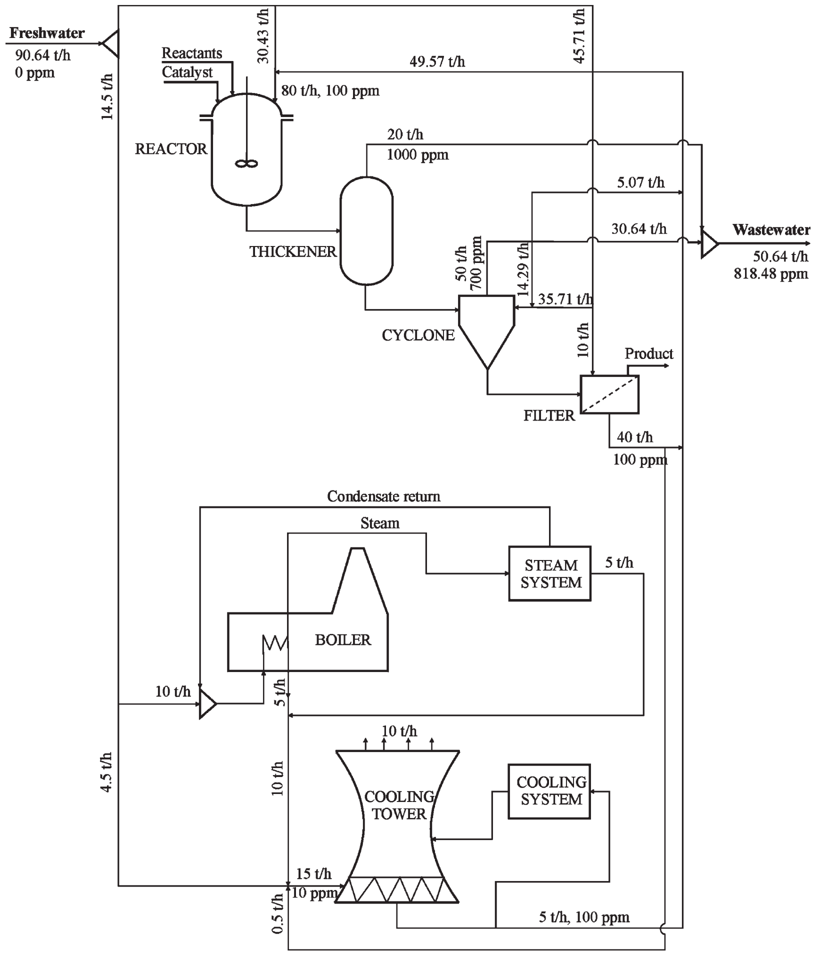

Figure 13. Optimal design of water network for specialty chemical plant (Example 3).

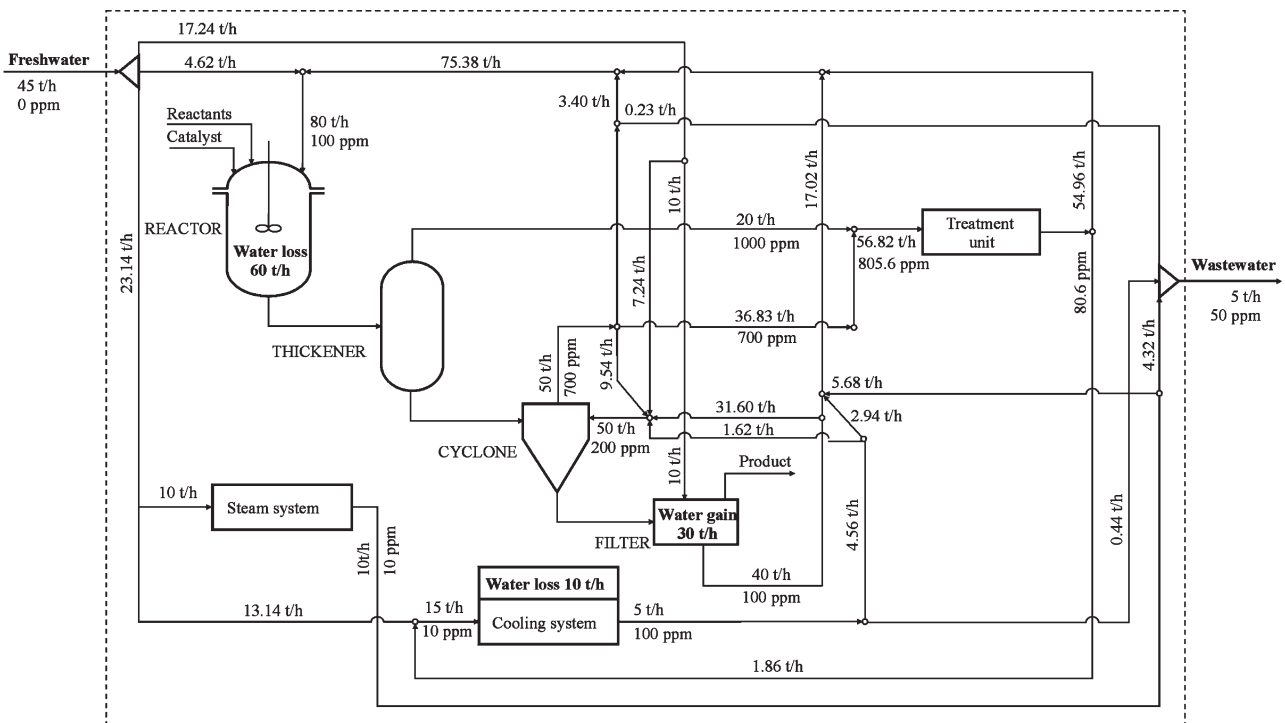

Figure 14. Optimal design of water network for specialty chemical plant by simultaneous optimization with local recycle (Example 3).

Table 10. Data for Water Sources (Example 4)

Water Source	Cost of Water Source ($/t)	Concentration of Contaminants (ppm)		
		A	*B*	*C*
SW_1	1.00	0	0	0
SW_2	0.50	25	35	35
SW_3	0.20	45	40	40
SW_4	0.15	50	50	50

Table 11. Data for Process Units (Example 4)

Process Unit	Flowrate (t/h)	Discharge Load (kg/h)			Maximum Inlet Concentration (ppm)		
		A	*B*	*C*	*A*	*B*	*C*
PU_1	40	1	1.5	1	25	25	25
PU_2	50	1	1	1	50	50	50
PU_3	60	1	1	1	50	50	50
PU_4	70	2	2	2	50	50	50
PU_5	80	1	1	0	25	25	25
PU_6	90	1	1	0	10	10	10

network to avoid that the derivatives become unbounded when the flows take zero values in the cost terms of the objective function.

The optimal solution ($1064078.1/year) for directly solving the MINLP is obtained in 197.5 CPUs (see Figure 16). It should be noted that the tolerance ε selected for the investment cost of the pipes in the network introduces very small error (7.8×10^{-6}) in the objective function while leading to

Table 12. Data for Treatment Units (Example 4)

Unit	Percentage Removal of Contaminant			IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
	A	*B*	*C*			
TU_1	95	0	0	16,800	1	0.7
TU_2	0	0	95	9500	0.04	0.7
TU_3	0	95	0	12,600	0.0067	0.7

bounded gradients for zero flows. The optimal number of removable piping connections in the network was 20.

Also, we solved the same problem using the two-stage solution strategy. The tolerance ε was selected to be 0.001 in the cost function for the investment cost of the pipes and the treatment units. First we solved the relaxed MINLP and the solution $1062741.89/year is obtained in 96.2 CPUs. Then, the 0–1 variables of streams in the network with zero value we fixed at zero and solved the reduced MINLP. The optimal solution $1062742.65/year of the reduced MINLP is obtained in 0.27 CPUs and contains 22 removable steams. The optimality gap of the reduced and the relaxed solution is only 7.2×10^{-6}. Furthermore, in this case, the total cost is somewhat smaller than in the case of the direct MINLP solution ($1062742.65/year vs. $1064078.1/year, i.e., 0.1% difference). This is because of the 0.01 optimality tolerance used in BARON.

To establish trade-offs between the network cost and network complexity we solved directly the corresponding MINLP problem by successively reducing the number of connections in the network. Results of the optimization are given in Figure 17, which shows the costs of the water

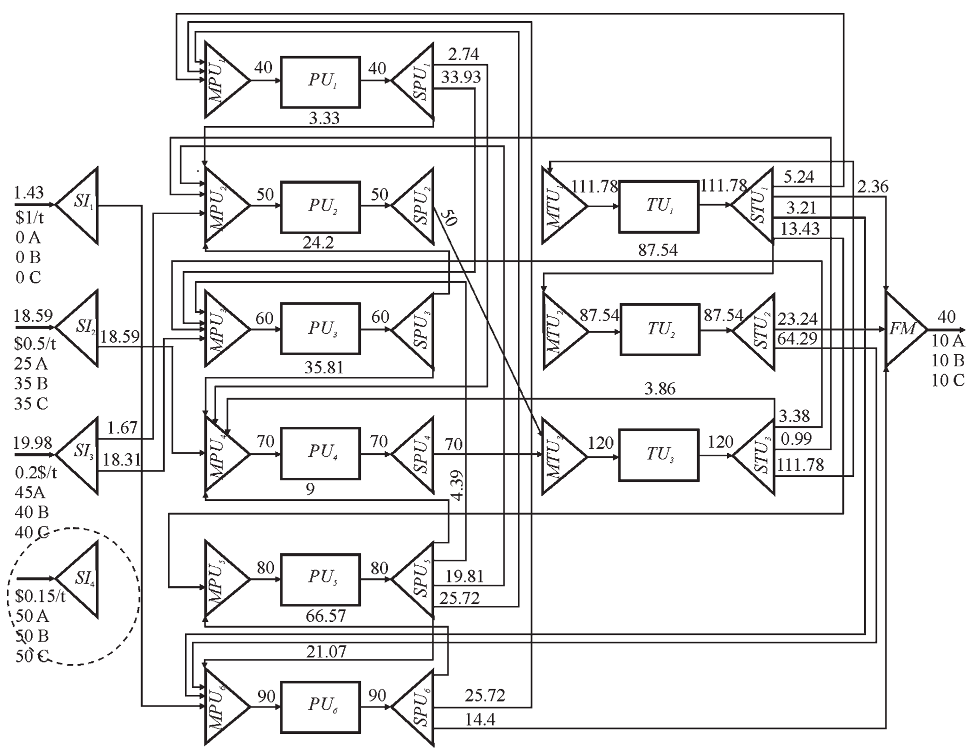

Figure 15. Optimal design of the integrated process network for Example 4.

Table 13. Data for Process Units (Example 5)

Processunit	Flowrate (t/h)	Discharge Load (kg/h)			Maximum Inlet Concentration (ppm)		
		A	*B*	*C*	*A*	*B*	*C*
PU_1	40	1	1.5	1	0	0	0
PU_2	50	1	1	1	50	50	50
PU_3	60	1	1	1	50	50	50
PU_4	70	2	2	2	50	50	50
PU_5	80	1	1	0	25	25	25

Table 14. Data for Treatment Units (Example 5)

Unit	Percentage Removal of Contaminant			IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
	A	*B*	*C*			
TU_1	95	0	0	16,800	1	0.7
TU_2	0	0	95	9500	0.04	0.7
TU_3	0	95	0	12,600	0.0067	0.7

networks for different number of removable connections. It is interesting to note that the freshwater consumption in all cases of Figure 17 was the same (40 t/h). The total computational time to generate the Pareto-optimal solutions of Figure 17 was 595 CPUs. In addition, it should be mentioned that the simplest water network has 13 removable connections and is shown in Figure 18. The total network cost for this case was \$1362882.5/year which is about 28% increase in the value of objective function compared to the optimal base case with 20 removable connections shown in Figure 16. However, the consumption of freshwater is the same as the one in Figure 16 (40 t/h). The increase in cost is due to the increased flows through the treatment units.

We also solved this MINLP example for the case when the flowrate through process units is allowed to be a continuous variable to be determined by the optimization (see Table 15). The optimality tolerance selected with BARON for optimization was 0.01. The optimal solution (\$1059826.41/year) of water network with 19 removable connections is obtained in 350 CPUs. The flowrates through process units (PU_1–PU_5) determined by optimization were as follows: 40, 27.81, 17.72, 70, and 34.20 t/h. As can be noticed, the computational time for solving this example was larger than in the case of solving the same MINLP problem with the fixed flowrate (197.5 CPUs). The main reason for this is the increased feasible space as well as the additional bilinear terms for the splitter and mixer of process units.

Example 6

This example illustrates the different possibilities for reducing the water consumption and the total costs for the network consisting of the water pre-treatment subsystem, the water-using subsystem, and the wastewater treatment subsystem. Moreover, we present results of the complete water integration, and zero liquid discharge cycles when all feasible interconnections between previously mentioned subsystems are allowed in the network.

Tables 16 and 17 show the data for this example that involves two process units (PU_1 and PU_2), two water pre-treatment units (TU_1 and TU_2), one wastewater treatment unit (TU_3), and four contaminants.

Data for the operating cost and the investment cost of the water pre-treatment (TU_1 and TU_2) and the wastewater treatment (TU_3) units are given in Table 17 and they are taken from Faria and Bagajewicz.[40]

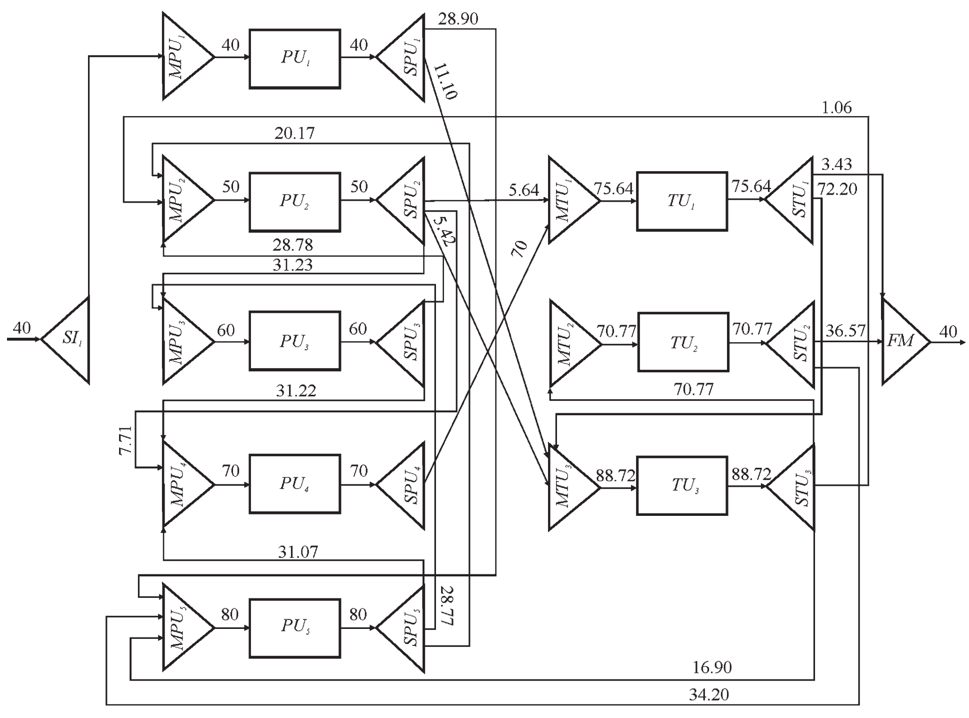

Figure 16. Optimal design of the water network with 20 removable connections (Example 5).

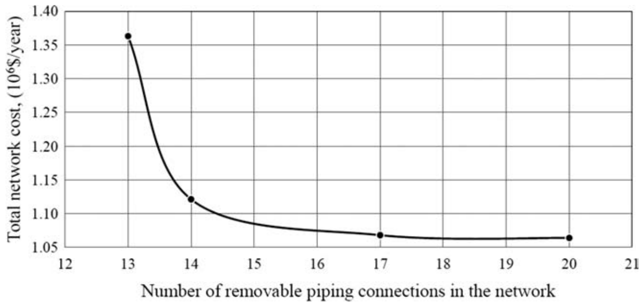

Figure 17. Costs of the water network for different number of removable connections (Example 5).

There is one freshwater source with four contaminants (100 ppm A, 100 ppm B, 100 ppm C, and 100 ppm D). The freshwater cost is assumed to be \$0.1/ton. The annualized factor for investment of the treatment units is assumed to be 0.1, and the total time for the network operation in a year 8600 h. The environmental discharge limit for all contaminants (A–D) concentration is 10 ppm. In addition, the maximum inlet contaminants concentration of the water pre-treatment unit TU_1 is 100 ppm and TU_2 10 ppm. We assume that the water pre-treatment units can purify the freshwater to the water quality down to 10 ppm for each contaminant (TU_1) and down to 0 ppm (TU_2). The percent removal of contaminants in the wastewater treatment unit (TU_3) was 95%. We used BARON to directly solve the MINLP in this example to global optimality. The optimality tolerance selected for optimization was zero.

Figure 19 shows the optimal design of water network when the recycling water from the water-using subsystem and the wastewater treatment subsystem is not allowed. The freshwater consumption is 50 t/h and the total network cost \$1244299.7/year.

In the next case shown in Figure 20, we assume that recycling water from the water-using and the wastewater treatment subsystem to the water pre-treatment subsystem is allowed. Note that the freshwater consumption is reduced to 40 t/h compared to the previous case. In addition, the total network cost is lower, \$1223838.0/year.

As can be seen from Figure 20, the network has the recycles from the water-using unit 2 (1.5 t/h) and from the

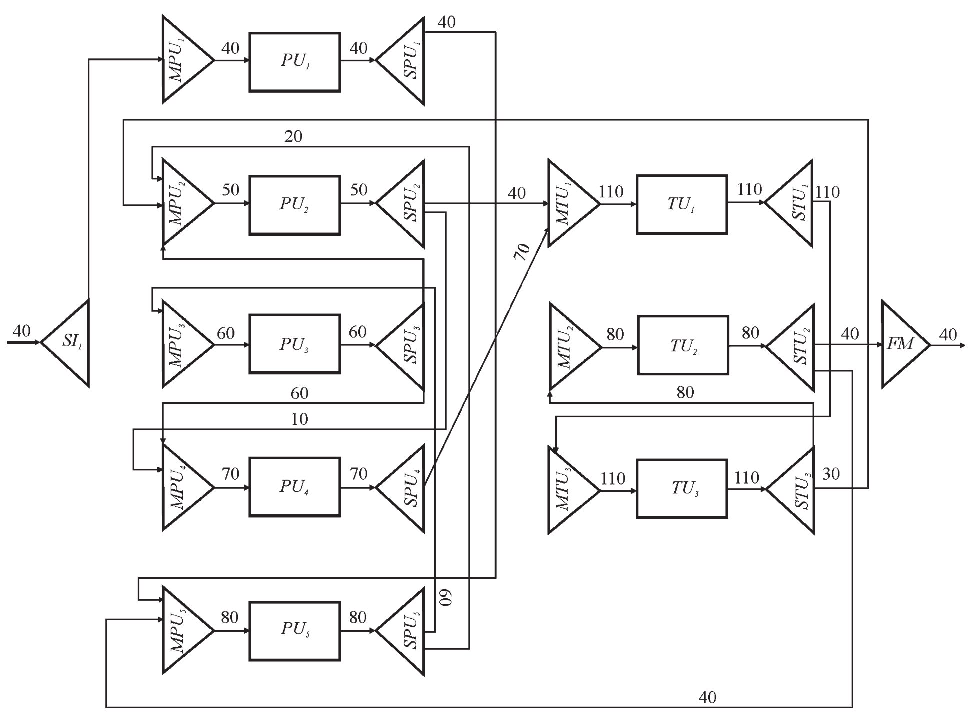

Figure 18. Optimal design of the simplified water network with 13 removable connections (Example 5).

Table 15. Data for the Variable Flowrates Through the Process Units (Example 5)

	Discharge Load (kg/h)			Maximum Inlet Concentration (ppm)			Maximum Outlet Concentration (ppm)			
Process Unit	*A*	*B*	*C*	*A*	*B*	*C*	*A*	*B*	*C*	Limiting Water Flowrate (t/h)
PU_1	1	1.5	1	0	0	0	25	37.5	25	40
PU_2	1	1	1	50	50	50	70	70	70	50
PU_3	1	1	1	50	50	50	66.67	66.67	66.67	60
PU_4	2	2	2	50	50	50	78.57	78.57	78.57	70
PU_5	1	1	0	25	25	25	37.5	37.5	25	80

Table 16. Data for Process Units (Example 6)

Unit	Flowrate (t/h)	Discharge Load (kg/h)				Maximum Inlet Concentration (ppm)			
		A	*B*	*C*	*D*	*A*	*B*	*C*	*D*
PU_1	40	1	1.5	1	1	0	0	0	0
PU_2	50	1	1	1	1	50	50	50	50

Table 17. Data for Pretreatment and Treatment Units (Example 6)

Unit	IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
TU_1 (Pretreatment 1)	10,000	0.10	0.7
TU_2 (Pretreatment 2)	25,000	1.15	0.7
TU_3 (Wastewater treatment)	30,000	1.80	0.7

wastewater treatment unit 3 (8.5 t/h) to the water pre-treatment unit 2. In addition, both types of freshwater (10 ppm and 0 ppm) are used in the network. The optimal design of water network with local recycle is shown in Figure 21. The total network cost is \$1057659.3/year and the freshwater consumption is the same (40 t/h) as in Figure 20, while the wastewater flowrate of treatment unit 3 is reduced from 42.5 t/h to 32.28 t/h.

It is worth pointing out that water networks can have zero liquid discharge cycles when all connections between the subsystems in the network are allowed (the complete water integration).

In Figure 22, we present the optimal network designs with zero liquid discharge cycles for this example. The total network cost for option without local recycle is \$1157863.5/year and for option with local recycle \$971320.7/year. Note that we assumed to have two pre-treatment units, but just one (TU_2) is selected by the optimization. Note also that although the use of freshwater has been eliminated the cost of treatment in Figure 22a is higher due to its higher flowrate (43.77 t/h vs. 32.28 t/h).

Model Sizes and Computational Times for Examples 1–6

Table 18 shows the sizes and computational times for the examples presented in the previous section. As can be seen from this table we solved NLP and MINLP problems of different sizes and complexity. The optimality tolerance selected for the global optimization in the first, third, and sixth example was 0.0 and in the second and fifth 0.01 and fourth 0.05. Also, all MINLP examples shown in Table 18 are directly solved. To solve the water network examples to global optimality we used the BARON solver. The computational times, for problems with and with no constraints on the removable streams were reasonable in all cases (see Table 18), although, it should be mentioned that by increasing the size of the NLP and MINLP problems computational time increases. This is especially true in Example 4 where changing the tolerance from 0.05 to 0.01 increases the CPU time from 2 CPUs to more than 5000 CPUs. It is worth to pointing out that we have also solved Example 4 using the local SNOPT solver ($\varepsilon = 0.01$) and obtained the same global optimal solution (\$1149710.84/year) in 0.2 CPUs, although

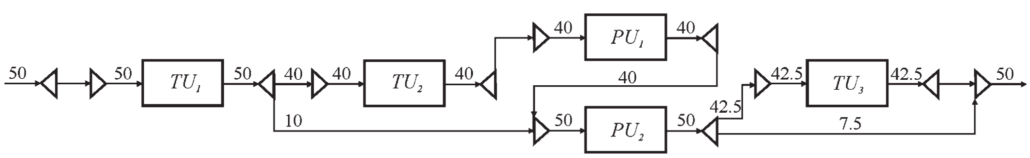

Figure 19. Recycling water from the water-using/wastewater treatment subsystem to the water pre-treatment subsystem is not allowed (Example 6).

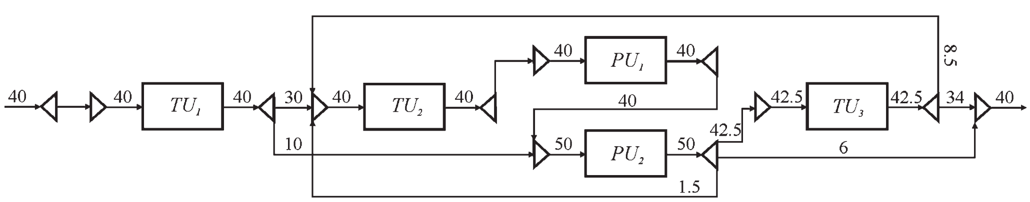

Figure 20. Recycling water from the water-using/wastewater treatment subsystem to the water pre-treatment subsystem is allowed (Example 6).

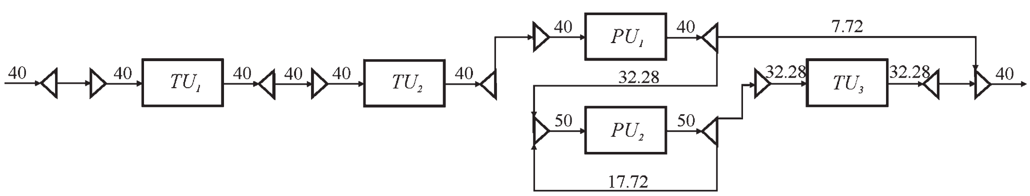

Figure 21. Optimal design of water network with local recycle (Example 6).

in this case global optimality cannot be guaranteed as the solution depends on the starting point.

In addition, we have directly solved the large-scale MINLP problem (Example 5) using the EMP and DICOPT solvers, which rely on convexity assumptions and, therefore, do not guarantee global optimality. Using EMP, the optimal solution ($1062703.09/year) is obtained in less than 1 CPUs while the optimal solution ($1064181.51/year) using DICOPT is obtained in less than 0.5 CPUs. These solutions are virtually identical to the one found by BARON with 0.01 optimality tolerance (($1064078.1/year).

Conclusions

In this article, we have presented a general superstructure and a global optimization strategy for the design of integrated process water network as well as its separate subsystems. The superstructure is quite general in that it includes all feasible interconnections in the network, mass transfer and non-mass transfer water-using processes, wastewater treatment operations, single and multiple sources of water with/without contaminants, and their possible pre-treatment. On the basis of this superstructure, we have formulated nonconvex NLP and MINLP models. The cost of piping and the cost of pumping water are included in the MINLP model. To solve more effectively the global optimization search of the proposed NLP and MINLP models, we have derived tight bounds on the variables as general equations obtained by physical inspection of the superstructure, and incorporated the cut by Karuppiah and Grossmann[1] to obtain tight lower bounds on the objective. Furthermore, we described a two-stage procedure for solving large-scale MINLP models.

From the examples, it is clear that the proposed approach can be successfully used for solving industrial water network problems as well as for establishing optimal trade-offs between the network cost and network complexity. The capabilities of the proposed method were illustrated on several examples, including large-scale water network problems. All the examples were solved to global optimality with reasonable computational time.

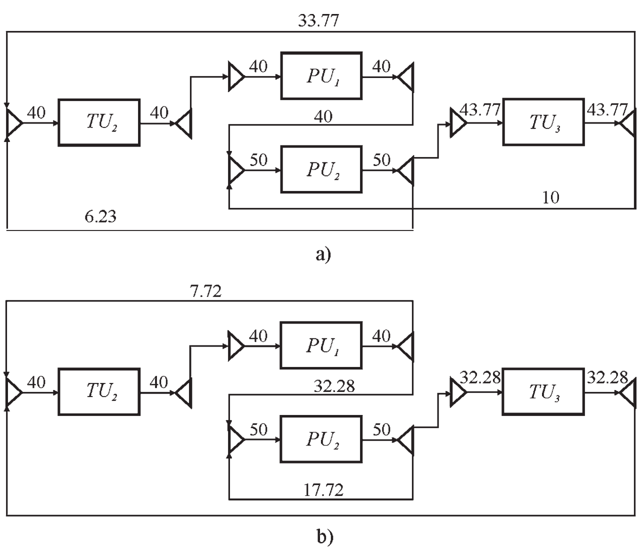

Figure 22. Optimal design of water network with zero liquid discharge cycles.

(a) Without local recycle. (b) With local recycle (Example 6).

Table 18. Model Statistics and Computational Results for Examples 1–6

Example	Number of Units	Continuous Variables	Discrete Variables	Constraints	CPU Time (s)
1	2PU-2TU	55	–	44	<0.5
		57*	–	44	<1.0
		75	20	85	<3.6
		79*	22	89	<2.5
		77**	20	85	13.2
2	2PU-2TU	57*	–	44	<0.5
	3PU-3TU	92	–	62	<0.5
	4PU-2PU	91	–	62	<0.5
	5PU-3TU	161	–	106	16.2
3	5PU	82	–	41	<0.5
	5PU-2TU	119	–	53	2.9
		126*	–	53	<0.5
4	6PU-3TU	223[a]	–	121	2.0
		223[b]	–	121	5874
5	5PU-3TU	233	72	251	197.5
		238**	72	251	350
6	2PU-3TU	135	30	148	<10.2
		145*	35	158	<0.6

*Option with local recycles.
**Variable flowrates in process units.
Optimality tolerances: 0.0 in Examples 1, 3, 6; 0.01 in Examples 2 and 5; in Example 4 a: 0.05, b: 0.01.

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Notation

Sets and indices

j = contaminant
DU = set of demand units
d = demand unit
PU = set of process units
p = process unit
SU = set of source units
r = source unit
SW = set of freshwater sources
s = freshwater source
TU = set of treatment units
t = treatment unit

Parameters

AR = annualized factor for investment for treatment units
CFW_s = cost of freshwater from source s
CP = fixed cost for each individual pipe in the network
$\mathrm{FDU}_d^{\mathrm{in}}$ = mass flowrate of inlet water stream in demand unit d
$\mathrm{FPU}_p^{\mathrm{in}}$ = mass flowrate of inlet water stream in process unit p
$\mathrm{FSU}_r^{\mathrm{out}}$ = mass flowrate of outlet water stream from source unit r
FWW_s = mass flowrate of freshwater source s
H = hours of plant operation per annum
IC_t = investment cost coefficient for treatment unit t
IP = variable cost for each individual pipe in the network
$\mathrm{LPU}_{p,j}$ = load of contaminant j in process unit p
$N_{\max}$ = maximum number of streams for the network
OC_t = operating cost coefficient for treatment unit t

PM = operating cost coefficient for pumping water through each pipe in the network

R_p, R_t = local recycle around process unit p and treatment unit t ($R_p = 0$ and $R_t = 0$ does not exist, $R_p = 1$ and $R_t = 1$ if exists)

$\mathrm{RR}_{t,j}$ = % removal of contaminant j in treatment unit t

$x_j^{\mathrm{out,max}}$ = maximum concentration of contaminant j in discharge stream to the environment

$x\mathrm{DU}_{d,j}^{\mathrm{in,max}}$ = maximum concentration of contaminant j in inlet stream into demand unit d

$x\mathrm{PU}_{p,j}^{\mathrm{in,max}}$ = maximum concentration of contaminant j in inlet stream into process unit p

$x\mathrm{SU}_{r,j}^{\mathrm{out}}$ = concentration of contaminant j in outlet stream from source unit r

$x\mathrm{W}_{s,j}^{\mathrm{in}}$ = concentration of contaminant j in freshwater source s

α = cost exponent for treatment units ($0 \leq \alpha \leq 1$)

$\beta_{\mathrm{TU}t,j}$ = $1-(\mathrm{RR}_{t,j}/100)$

γ = cost exponent for pipes ($0 \leq \gamma \leq 1$)

Continuous variables

F^{out} = mass flowrate of outlet wastewater stream from final mixer

$\mathrm{FID}_{s,d}$ = mass flowrate of water stream from freshwater source s to demand unit d

FIF_s = mass flowrate of water stream from freshwater source s to final mixer

$\mathrm{FIP}_{s,p}$ = mass flowrate of water stream from freshwater source s to process unit p

$\mathrm{FIT}_{s,t}$ = mass flowrate of water stream from freshwater source s to treatment unit t

$\mathrm{FP}_{p',p}$ = mass flowrate of water stream from process unit p' to process unit p

$\mathrm{FPD}_{p,d}$ = mass flowrate of water stream from process unit p to demand unit d

FPO_p = mass flowrate of water stream from process unit p to final mixer

$\mathrm{FPT}_{p,t}$ = mass flowrate of water stream from process unit p to treatment unit t

$\mathrm{FPU}_p^{\mathrm{in}}$ = mass flowrate of inlet water stream in process unit p when treated as continuous variable

$\mathrm{FPU}_p^{\mathrm{out}}$ = mass flowrate of outlet water stream from process unit p when treated as continuous variable

$\mathrm{FSD}_{r,d}$ = mass flowrate of water stream from source unit r to demand unit d

FSO_r = mass flowrate of water stream from source unit r to final mixer

$\mathrm{FSP}_{r,p}$ = mass flowrate of water stream from source unit r to process unit p

$\mathrm{FST}_{r,t}$ = mass flowrate of water stream from source unit r to treatment unit t

$\mathrm{FT}_{t',t}$ = mass flowrate of water stream from treatment unit t' to treatment unit t

$\mathrm{FTD}_{t,d}$ = mass flowrate of water stream from treatment unit t to demand unit d

FTO_t = mass flowrate of water stream from treatment unit t to final mixer

$\mathrm{FTP}_{t,p}$ = mass flowrate of water stream from treatment unit t to process unit p

$\mathrm{FTU}_t^{\mathrm{in}}$ = mass flowrate of inlet water stream in treatment unit t

$\mathrm{FTU}_t^{\mathrm{out}}$ = mass flowrate of outlet water stream from treatment unit t

FW_s = mass flowrate of water for freshwater source s

x_j^{out} = concentration of contaminant j in discharge stream to the environment

$x\mathrm{DU}_{d,j}^{\mathrm{in}}$ = concentration of contaminant j in inlet stream into demand unit d

$x\mathrm{PU}_{p,j}^{\mathrm{in}}$ = concentration of contaminant j in inlet stream into process unit p

$x\mathrm{PU}_{p,j}^{\mathrm{out}}$ = concentration of contaminant j in outlet stream from process unit p

$x\mathrm{SPU}_{t,j}^{\mathrm{out}}$ = concentration of contaminant j in outlet stream from splitter process unit p

$x\mathrm{STU}_{t,j}^{\mathrm{out}}$ = concentration of contaminant j in outlet stream from splitter treatment unit t

$x\mathrm{TU}_{t,j}^{\mathrm{in}}$ = concentration of contaminant j in inlet stream into treatment unit t

$x\mathrm{TU}_{t,j}^{\mathrm{out}}$ = concentration of contaminant j in outlet stream from treatment unit t

Binary variables

$y_{\mathrm{FID}_{s,d}}$ = existence of pipe between freshwater source s and demand unit d

y_{FIF_s} = existence of pipe between freshwater source s and final mixer

$y_{\mathrm{FIP}_{s,p}}$ = existence of pipe between freshwater source s and process unit p

$y_{\mathrm{FIT}_{s,t}}$ = existence of pipe between freshwater source s and treatment unit t

$y_{\mathrm{FP}_{p',p}}$ = existence of pipe between process unit p' and process unit p

$y_{\mathrm{FPD}_{p,d}}$ = existence of pipe between process unit p and demand unit d

y_{FPO_p} = existence of pipe between process unit p and final mixer

$y_{\mathrm{FPT}_{p,t}}$ = existence of pipe between process unit p and treatment unit t

$y_{\mathrm{FSD}_{r,d}}$ = existence of pipe between source unit r and demand unit d

y_{FSO_r} = existence of pipe between source unit r and final mixer

$y_{\mathrm{FSP}_{r,p}}$ = existence of pipe between source unit r and process unit p

$y_{\mathrm{FST}_{r,t}}$ = existence of pipe between source unit r and treatment unit t

$y_{\mathrm{FT}_{t',t}}$ = existence of pipe between treatment unit t' and treatment unit t

$y_{\mathrm{FTD}_{t,d}}$ = existence of pipe between treatment unit t and demand unit d

y_{FTO_t} = existence of pipe between treatment unit t and final mixer

$y_{\mathrm{FTP}_{t,p}}$ = existence of pipe between treatment unit t and process unit p

Subscripts/Superscripts

FX = fixed bound for the variable

in = inlet stream

L = lower bound for the variable

max = maximal

out = outlet stream

U = upper bound for the variable

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Appendix

Variable bounds for the proposed model

In the proposed NLP/MINLP optimization model, the bounds on the variables are represented as general equations in this appendix. The model and the bounds can be used to address both classes of water network problems with the fixed and variable flowrate through the water-using units. In the second one, the variable flowrate presents a continuous variable to be determined by the optimization. In this appendix, variable bounds are presented for the fixed as well as variable flowrate through the water-using units.

Initial splitter

The upper bound of water flowrate at the initial splitter can be determined on the basis of fixed flowrates for all process and demand units.

$$\mathrm{FW}_s^{\mathrm{U}} = \sum_{p\in\mathrm{PU}} \mathrm{FPU}_p^{\mathrm{in}} + \sum_{d\in\mathrm{DU}} \mathrm{FDU}_d^{\mathrm{in}} \qquad \forall s\in\mathrm{SW},\ |\mathrm{PU}|\neq 0. \tag{A1}$$

The lower bound of the water flowrate at the initial splitter has a minimum fixed flowrate for a process unit if one external source of water exists in the network. If there are more sources of water in the network, the lower bound is set to be zero because it is possible that some sources of water will not be selected by the optimization model.

$$\mathrm{FW}_s^{\mathrm{L}} = \min_p \left(\mathrm{FPU}_p^{\mathrm{in}}\right) \qquad \forall s\in\mathrm{SW},\ |\mathrm{PU}|\neq 0\,,\ |\mathrm{SW}| = 1. \tag{A2}$$

The upper bound for flowrates going from the initial splitter to the mixer treatment units can be determined on the basis of fix flowrates for all process units.

$$\mathrm{FIT}_{s,t}^{\mathrm{U}} = \sum_{p\in\mathrm{PU}} \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall s\in\mathrm{SW}, \forall t\in\mathrm{TU},\ |\mathrm{PU}|\neq 0. \tag{A3}$$

In the case that the water network consists only of treatment units (number of process units is set to be zero), then wastewater feed flowrates are fixed and the upper bounds of flowrates from the initial splitter to the mixer treatment units and the final mixer are given as follows.

$$\mathrm{FW}_s^{FX} = \mathrm{FWW}_s^{\mathrm{in}} \qquad \forall s\in\mathrm{SW},\ |\mathrm{PU}| = 0. \tag{A4}$$

$$\mathrm{FIT}_{s,t}^{\mathrm{U}} = \mathrm{FWW}_s^{\mathrm{in}} \qquad \forall s\in\mathrm{SW}, \forall t\in\mathrm{TU},\ |\mathrm{PU}| = 0 \tag{A5}$$

$$\mathrm{FIF}_s^{\mathrm{U}} = \mathrm{FWW}_s^{\mathrm{in}} \qquad \forall s\in\mathrm{SW},\ |\mathrm{PU}| = 0. \tag{A6}$$

The upper bound of water flowrate going from the initial splitter to the process units depends of the fixed flowrate in particular process units.

$$\mathrm{FIP}_{s,p}^{\mathrm{U}} = \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall s\in\mathrm{SW}, \forall p\in\mathrm{PU}. \tag{A7}$$

Process units

The process units can be considered as part of the integrated water network, as well as a separate water-using subsystem. The inlet and outlet flowrates of the process unit are the same. For class of water network problems with the fixed flowrate through the process unit, the outlet flowrate of the process unit has fixed value and depends of the inlet flowrate.

$$\mathrm{FPU}_p^{\mathrm{out}^{FX}} = \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p \in \mathrm{PU}. \tag{A8}$$

For water network problems with variable flowrates through the process units, on the basis of data given (the maximum inlet and outlet contaminant concentration, and the mass load of contaminant) the limiting water flowrate can be calculated as given by Eq. A8a. This flowrate presents the flowrate required if the specified mass of contaminant is picked up by the water between the maximum inlet and outlet concentration.

$$\mathrm{FPU}_p^{\mathrm{out}^{\mathrm{MAX}}} = \frac{\mathrm{LPU}_{p,j}}{x\mathrm{PU}_{p,j}^{\mathrm{out,max}} - x\mathrm{PU}_{p,j}^{in,\mathrm{max}}} \qquad \forall p \in \mathrm{PU}, \forall j. \tag{A8a}$$

The upper bound for the inlet and outlet flowrate of the process unit depends of the limiting water flowrate as follows.

$$\mathrm{FPU}_p^{\mathrm{in}^U} = \mathrm{FPU}_p^{\mathrm{out}^{\mathrm{MAX}}} \qquad \forall p \in \mathrm{PU} \tag{A8b}$$

$$\mathrm{FPU}_p^{\mathrm{out}^U} = \mathrm{FPU}_p^{\mathrm{out}^{\mathrm{MAX}}} \qquad \forall p \in \mathrm{PU}. \tag{A8c}$$

In addition, this limiting flowrate is used in other equations in Appendix to calculate bounds instead of the specified value ($\mathrm{FPU}_p^{\mathrm{in}}$) for the water network problems with fixed flowrate through process units.

The upper and lower bounds for contaminants concentration at the process unit inlets and outlets are given as follows.

$$x\mathrm{PU}_{p,j}^{\mathrm{in}^{\mathrm{U}}} = x\mathrm{PU}_{p,j}^{\mathrm{in,max}} \qquad \forall p \in \mathrm{PU}, \forall j \tag{A9}$$

$$x\mathrm{PU}_{p,j}^{\mathrm{in}^{\mathrm{L}}} = \mathrm{LPU}_{p,j}/\mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p \in \mathrm{PU}, \forall j \tag{A10}$$

$$x\mathrm{PU}_{p,j}^{\mathrm{out}^{\mathrm{U}}} = (x\mathrm{PU}_{p,j}^{\mathrm{in,max}} \cdot \mathrm{FPU}_p^{\mathrm{in}} + \mathrm{LPU}_{p,j})/\mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p \in \mathrm{PU}, \forall j. \tag{A11}$$

In the case of water problems with variable flowrates through the process units, the upper bound for contaminants concentration are given by Eqs. A11a, A14a, A21a, and A43a.

$$x\mathrm{PU}_{p,j}^{\mathrm{out}^U} = x\mathrm{PU}_{p,j}^{\mathrm{out,max}} \qquad \forall p \in \mathrm{PU}, \forall j. \tag{A11a}$$

Splitter process units

The splitter process units streams can be directed to any mixer process units so the upper bounds of these flowrates depend of the fixed flowrates in a particular process unit. Notice that the outlet contaminants concentration of the process unit and the splitter process unit are the same.

$$\mathrm{FP}_{p',p}^{\mathrm{U}} = \mathrm{FPU}_p^{\mathrm{in}} \quad \text{if } \mathrm{FPU}_{p'}^{\mathrm{in}} \le \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p' \in \mathrm{PU}, \forall p \in \mathrm{PU} \tag{A12}$$

$$\mathrm{FP}_{p',p}^{\mathrm{U}} = \mathrm{FPU}_p^{\mathrm{in}} \quad \text{if } \mathrm{FPU}_{p'}^{\mathrm{in}} \ge \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p' \in \mathrm{PU}, \forall p \in \mathrm{PU} \tag{A13}$$

$$x\mathrm{SPU}_{p,j}^{\mathrm{out}^U} = x\mathrm{PU}_{p,j}^{\mathrm{out}} \qquad \forall p \in \mathrm{PU}, \forall j \tag{A14}$$

$$x\mathrm{SPU}_{p,j}^{\mathrm{out}^{\mathrm{U}}} = x\mathrm{PU}_{p,j}^{\mathrm{out,max}} \qquad \forall p \in \mathrm{PU}, \forall j. \tag{A14a}$$

The upper bounds for flowrates going from the splitter process units to the mixer treatment units and the final mixer depend of the fixed flowrates of process units.

$$\mathrm{FPT}_{p,t}^{\mathrm{U}} = \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p \in \mathrm{PU}, \forall t \in \mathrm{TU} \tag{A15}$$

$$\mathrm{FPO}_p^{\mathrm{U}} = \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall p \in \mathrm{PU}. \tag{A16}$$

Treatment units

The treatment units can be considered as part of the integrated water network, as well as a separate wastewater subsystem. According to this, the upper bounds for flowrates and contaminants concentration of the treatment units are given as follows.

$$\mathrm{FTU}_t^{\mathrm{in}^{\mathrm{U}}} = \sum_{p \in \mathrm{PU}} \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall t \in \mathrm{TU}, |\mathrm{PU}| \ne 0 \tag{A17}$$

$$\mathrm{FTU}_t^{\mathrm{in}^{\mathrm{U}}} = \sum_{s \in \mathrm{SW}} \mathrm{FWW}_s^{\mathrm{in}} \qquad \forall t \in \mathrm{TU}, |\mathrm{PU}| = 0 \tag{A18}$$

$$\mathrm{FTU}_t^{\mathrm{out}^{\mathrm{U}}} = \sum_{p \in \mathrm{PU}} \mathrm{FPU}_p^{\mathrm{in}} \qquad \forall t \in \mathrm{TU}, |\mathrm{PU}| \ne 0 \tag{A19}$$

$$\mathrm{FTU}_t^{\mathrm{out}^{\mathrm{U}}} = \sum_{s \in \mathrm{SW}} \mathrm{FWW}_s^{\mathrm{in}} \qquad \forall t \in \mathrm{TU}, |\mathrm{PU}| = 0 \tag{A20}$$

$$x\mathrm{TU}_{t,j}^{\mathrm{in}^{\mathrm{U}}} = \max_{p \in \mathrm{PU}} \left[(x\mathrm{PU}_{p,j}^{\mathrm{in,max}} \cdot \mathrm{FPU}_p^{\mathrm{in}} + \mathrm{LPU}_{p,j})/\mathrm{FPU}_p^{\mathrm{in}} \right] \qquad \forall t \in \mathrm{TU}, \forall j,\ |\mathrm{PU}| \ne 0 \tag{A21}$$

$$x\mathrm{TU}_{t,j}^{\mathrm{in}^{\mathrm{U}}} = \max_{p \in \mathrm{PU}} (x\mathrm{PU}_{p,j}^{\mathrm{out,max}}) \quad \forall t \in \mathrm{TU}, \forall j,\ |\mathrm{PU}| \ne 0 \tag{A21a}$$

$$x\mathrm{TU}_{t,j}^{\mathrm{in}^{\mathrm{U}}} = \max_{s \in \mathrm{SW}} (x\mathrm{W}_{s,j}^{\mathrm{in}}) \qquad \forall t \in \mathrm{TU}, \forall j, |\,\mathrm{PU}| = 0 \tag{A22}$$

$$x\mathrm{TU}_{t,j}^{\mathrm{out}^{\mathrm{U}}} = (1 - \mathrm{RR}_{t,j}/100) \cdot x\mathrm{TU}_{t,j}^{\mathrm{in}^{\mathrm{U}}} \qquad \forall t \in \mathrm{TU}, \forall j. \tag{A23}$$

Splitter treatment units

The streams from splitter process units can be directed to any mixer in the network. The upper bounds of these streams are given as follows.

$$FT^{U}_{t',t} = \sum_{p\in PU} FPU^{in}_{p} \qquad \forall t' \in TU, \forall t \in TU, |PU| \neq 0 \quad (A24)$$

$$FT^{U}_{t',t} = \sum_{s\in SW} FWW^{in}_{s} \qquad \forall t' \in TU, \forall t \in TU, |PU| = 0 \quad (A25)$$

$$FTP^{U}_{t,p} = FPU^{in}_{p} \qquad \forall t \in TU, \forall p \in PU \qquad (A26)$$

$$FTO^{U}_{t} = \sum_{p\in PU} FPU^{in}_{p} \qquad \forall t \in TU, |PU| \neq 0 \qquad (A27)$$

$$FTO^{U}_{t} = \sum_{s\in SW} FWW^{in}_{s} \qquad \forall t \in TU, |PU| = 0 \qquad (A28)$$

$$xSTU^{out^{U}}_{t,j} = xTU^{out^{U}}_{t,j} \qquad \forall t \in TU, \forall j. \qquad (A29)$$

Source and demand units

It should be noted that inlet and outlet flowrates of water-using operations can have different values. In that case, they can be divided in two parts. The first part can be considered unchanged through process, and the second part can account for the loss of water or the gain of water. According to this, the upper bounds of flowrates and contaminants concentrations are given as follows.

$$FID^{U}_{s,d} = FDU^{in}_{d} \qquad \forall s \in SW, \forall d \in DU \qquad (A30)$$

$$xDU^{in^{U}}_{d,j} = xDU^{in,max}_{d,j} \qquad \forall d \in DU, \ \forall j \qquad (A31)$$

$$FPD^{U}_{p,d} = FDU^{in}_{d} \qquad \forall p \in PU, \forall d \in DU \qquad (A32)$$

$$FTD^{U}_{t,d} = FDU^{in}_{d} \qquad \forall t \in TU, \forall d \in DU \qquad (A33)$$

$$FST^{U}_{r,t} = \sum_{p\in PU} FPU^{in}_{p} \qquad \forall r \in SU, \forall t \in TU \qquad (A34)$$

$$FSO^{U}_{r} = FSU^{out}_{r} \qquad \forall r \in SU \qquad (A35)$$

$$FSD^{U}_{r,d} = FDU^{in}_{d} \qquad \forall r \in SU, \forall d \in DU \qquad (A36)$$

$$xSU^{in^{U}}_{r,j} = xSU^{in,max}_{r,j} \qquad \forall r \in SU, \ \forall j. \qquad (A37)$$

Final mixer

The lower bound of the discharge flowrate to the environment has a minimum value of the fixed flowrates in the process units. However, if the network consists only of treatment units then it has a minimum value of wastewater streams of the initial splitters.

$$F^{out\,L} = \min_{p\in PU} (FPU^{in}_{p}) \qquad |PU| \neq 0 \qquad (A38)$$

$$F^{out\,L} = \min_{s\in SW} (FWW^{in}_{s}) \qquad |PU| = 0 \qquad (A39)$$

The upper bounds of the discharge flowrate and contaminants concentration are given as follows.

$$F^{out^{U}} = \sum_{p\in PU} FPU^{in}_{p} \qquad |PU| \neq 0 \qquad (A40)$$

$$F^{out^{U}} = \sum_{s\in SW} FWW^{in}_{s} \qquad |PU| = 0 \qquad (A41)$$

$$x^{out^{U}}_{j} = x^{out,max}_{j} \qquad \forall j \qquad (A42)$$

$$x^{out^{U}}_{j} = \max_{p\in PU}\left[(xPU^{in,max}_{p,j} \cdot FPU^{in}_{p} + LPU_{p,j})/FPU^{in}_{p}\right] \qquad \forall j, \ |TU| = 0 \qquad (A43)$$

$$x^{out^{U}}_{j} = \max_{p\in PU}(xPU^{out,max}_{p,j}) \qquad \forall j, \ |TU| = 0 \qquad (A43a)$$

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