GLOBAL OPTIMIZATION FOR THE SYNTHESIS OF INTEGRATED WATER SYSTEMS IN CHEMICAL PROCESSES

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ABSTRACT

In this paper, we address the problem of optimal synthesis of an integrated water system, where water using processes and water treatment operations are combined into a single network such that the total cost of obtaining freshwater for use in the water using operations, and treating wastewater is minimized. A superstructure, which incorporates all feasible design alternatives for water treatment, reuse and recycle, is proposed. We formulate this structure as a non-convex Non-Linear Programming (NLP) problem, which is solved to global optimality. The problem takes the form of a non-convex Generalized Disjunctive Program (GDP) if there is a flexibility of choosing different treatment technologies for the removal of the various contaminants in the wastewater streams. A new deterministic spatial branch and contract algorithm is proposed for optimizing such systems, in which piecewise under- and over-estimators are used to approximate the non-convex terms in the original model to obtain a convex relaxation whose solution gives a lower bound on the global optimum. These lower bounds are made to converge to the solution within a branch and bound procedure. Several examples are presented to illustrate the optimization of these integrated networks using the proposed algorithm.

Keywords: Global optimization; Integrated water networks; Superstructure; Piecewise estimators

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1. Introduction

Water is one of the most important natural resources being used in the process industry (Dudley, 2003). For instance, it is used for desalting crude oil in petroleum refineries, for liquid-liquid extraction in hydrometallurgy, as a cooling, quenching and scrubbing agent in the iron and steel industry, and for a variety of washing operations in the food and agricultural industries. The predicted scarcities of industrial water over the next few decades and the increasingly stringent environmental regulations for wastewater disposal will require efficient and responsible utilization of water in industry.

Traditionally, freshwater has been used for process use, and the wastewater generated in these processes has been treated in a central common facility in order to remove contaminants to meet regulatory specifications for the wastewater disposal. As opposed to this conventional approach, reusing and re-routing the water streams in an integrated water network helps in reducing the consumption of freshwater in the system, and minimizes the amount of wastewater to be treated and disposed into the environment. This, in turn, brings down the cost of obtaining freshwater and also the cost of effluent treatment. Wang and Smith (1994a) have proposed water reuse, regeneration-reuse and regeneration-recycling as an approach for wastewater minimization. They have also proposed a methodology for designing effluent treatment systems where wastewater is treated in a distributed manner. Treating wastewater in a distributed way, in which effluent streams are treated separately instead of combining them into a single stream prior to treatment, reduces the treatment cost since the capital cost and operating cost of a treatment operation are directly proportional to the water flowrate through the treatment unit, which is smaller in the case of distributed systems (McLaughin et al., 1992).

Most of the studies published in literature have dealt with the issue of minimizing wastewater generation in water using processes, separately from the design of effluent treatment systems. A conceptual approach has been used by Wang and Smith (1994a) to minimize the wastewater generation in process industries. Feng and Seider (2001) have proposed a novel network structure with internal water mains to deal with the issue of reducing of water consumption and wastewater generation as well as to simplify the piping network in large plants. To the same end, Alva-Argaez et al. (1998) have used a mathematical programming approach to optimize a superstructure, which includes possibilities for water treatment and reuse. In their solution approach, they present a Mixed Integer Non-Linear Programming (MINLP) model, which is decomposed into a sequence of Mixed Integer Linear Programming (MILP) problems to approximate the optimal solution. Bagajewicz et al. (1999) proposed a method to transform the formulation of a multi-contaminant large scale water system from a non-linear program (NLP) to a linear program (LP) and solved it to optimality. Further, there have also been numerous studies in the past to address the problem of optimizing wastewater treatment networks. Graphical techniques have been presented by Kuo and Smith (1997) and by Wang and Smith (1994b) to set targets for the minimum flowrate in a distributed effluent system and to design such systems. Galan and Grossmann (1998) suggested an effective heuristic mathematical programming procedure for the optimal design of a distributed wastewater treatment network, where they optimize the superstructures given by Wang and Smith (1994b). The superstructure optimization problem was further extended by Lee and Grossmann (2003), who formulated the decentralized wastewater treatment network as a non-convex Generalized Disjunctive Program (GDP) and solved the problem to global optimality.

In contrast to these studies, there are very few studies on the integration of water using and treating processes into a single system. The seminal paper in this area was by Takama et al. (1980), who solved the problem of optimal water allocation in a petroleum refinery. They generated a superstructure allowing for all water reuse and regeneration possibilities, and then mathematically optimized it. Similar work has been done by Huang et al. (1999), who present a theoretical model for constructing an optimal *Water Usage and Treatment Network (WUTN)* in a chemical plant. In both of the above-mentioned works, the integrated networks were modeled as non-linear programming problems and then optimized. Global optimality is not guaranteed in either of them.

A comprehensive review of the various graphical and mathematical programming techniques to design and retrofit water networks is given in Bagajewicz (2000) where the author lists and compares the work done using these two approaches. The author also points out that this area of optimal water allocation and treatment is moving towards the use of mathematical programming techniques, because of the tedious nature of the graphical methods and their severe limitations in handling multicomponent systems.

In this paper, we generalize the synthesis problem by proposing a superstructure, similar to that by Takama et al. (1980), for the design of integrated water systems that combines the water using and water treating units in a single network. The superstructure, which incorporates all the feasible design alternatives for water treatment, reuse and recycle, is initially formulated as an NLP problem. Later in the paper, we allow for the selection of different technologies for treating wastewater, and thereby model the superstructure optimization as a GDP problem, which is then reformulated as a MINLP problem. The superstructure optimization models are non-convex due to the presence of bilinearities in the constraints and so the local NLP algorithms often fail to converge to a solution, or else lead to sub-optimal solutions. Similarly, the existing standard methods for solving MINLPs (see Grossmann, 2002), like Outer Approximation (OA) and Generalized Benders Decomposition (GBD), do not guarantee to find the global optimum for non-convex problems. Various deterministic global optimization techniques for solving non-convex NLPs with special structures in the continuous variables have been proposed, for instance by Quesada and Grossmann (1995a), Ryoo and Sahinidis (1995) and Zamora and Grossmann (1999). Additionally, excellent reviews on global optimization methods for solving non-convex NLP problems are given in Floudas (2000) and Horst and Tuy (1996). For addressing non-convexities in MINLPs, Adjiman et al. (2000), Kesavan and Barton (1999), Smith and Pantelides (1997) and Tawarmalani and Sahinidis (2001) have proposed various types of algorithms. Bergamini et al. (2004) and Lee and Grossmann (2001) have presented different global optimization algorithms for the case of GDP problems.

In this work, we propose a new spatial branch and contract algorithm for solving to global optimality, the non-convex NLP/ MINLP problems that arise in the synthesis of integrated water systems. Piecewise linear under- and over-estimators are used to approximate the non-convex terms in the original NLP/ MINLP, to obtain an MILP problem whose solution provides a tight lower bound at every node of the spatial branch and bound tree. These lower bounds are compared against the upper bounds (obtained by solving the non-convex NLP/ MINLP) in a branch and bound enumeration. Several examples are presented to illustrate that the proposed method requires a reasonable amount of time to solve, given the fact that general purpose spatial branch and bound methods can be computationally expensive.

2. Motivating Example

We consider a simple example in order to demonstrate the advantage of optimizing an integrated structure of water using and water treatment units over sequentially minimizing, first the freshwater consumed in the water using processes, and then the wastewater treated in the treatment units. We consider a system with two process units that use fixed amounts of water (PU1 and PU2), and construct a superstructure with all possible connections between these units. These units are also connected to a single freshwater source at the inlet of this system. Fixed loads of contaminants are assumed to be generated in each of the process units. This structure is shown in Fig. 1a, where the SU's and MU's denote the splitters and mixers respectively.

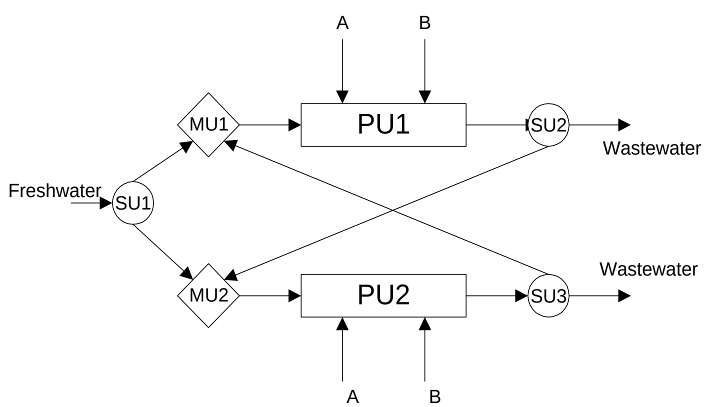

Fig. 1a Superstructure of a network with 2 Process Units

On globally optimizing this network with the data for the process units given in Table 1 (Section 7), the optimal freshwater consumption in this system is found to be 50 ton/hr. The optimized structure is shown in Fig 1b.

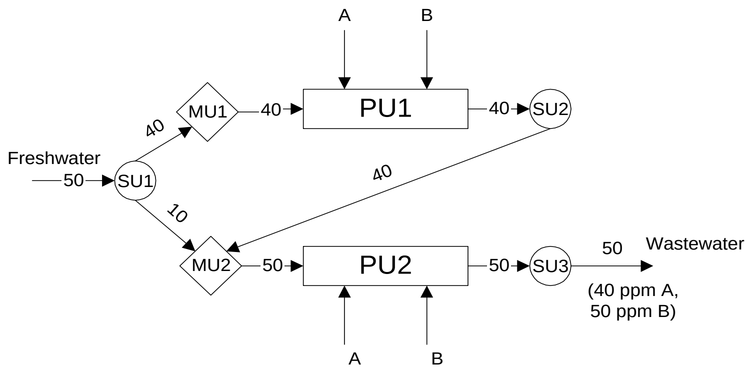

Fig. 1b Optimal structure of the network with 2 Process Units

Further, the effluent streams from this system are treated in a set of interconnected treatment units, TU1 and TU2, whose superstructure is presented in Fig. 2a. The contaminant removal ratios for TU1 and TU2 are given in Table 2, Section 7. After treatment, the effluent stream is discharged into the environment and the discharge limit for both contaminants A and B present in the stream is taken to be 10 ppm. The objective of the optimization problem here is to minimize the sum of the wastewater flows into both the treatment units. Fig. 2b shows the optimal network structure for the wastewater treatment.

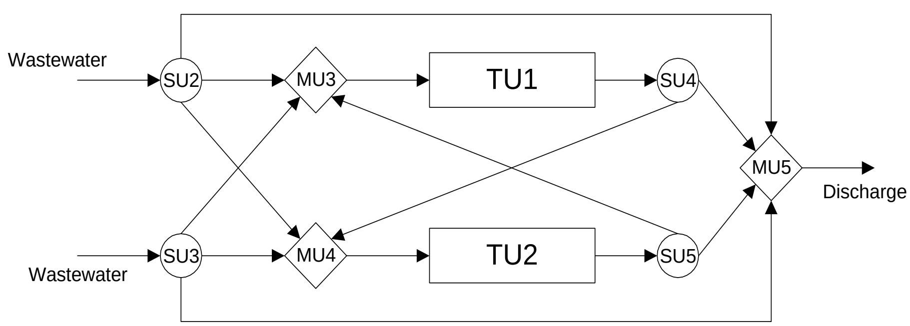

Fig. 2a Superstructure for a system with 2 Treatment Units

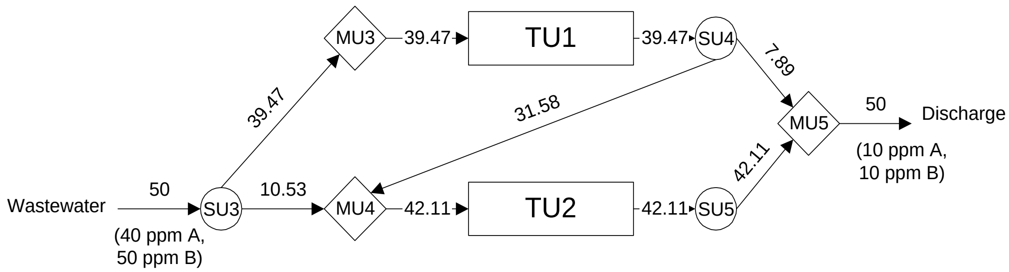

Fig. 2b Optimal network design for effluent treatment with 2 Treatment Units

As a result of this sequential optimization, the sum of the freshwater consumption in the water using processes and the wastewater flows handled by the treatment units is found to be 50 + 81.58 = 131.58 ton/hr. On simultaneously optimizing the integrated network (superstructure given in Fig. 3a), instead of independently optimizing the structures for water using processes and the water treating operations, the sum of the freshwater consumed in the system and the wastewater treated in the treatment units in the optimal network (Fig. 3b) reduces to 117.05 ton/hr, which is an 11 % improvement over the result obtained from sequential optimization. Moreover, the consumption of freshwater is reduced from 50 ton/ hr to 40 ton/ hr. Thus, it is clear that the benefits of an integrated optimization approach can be very significant.

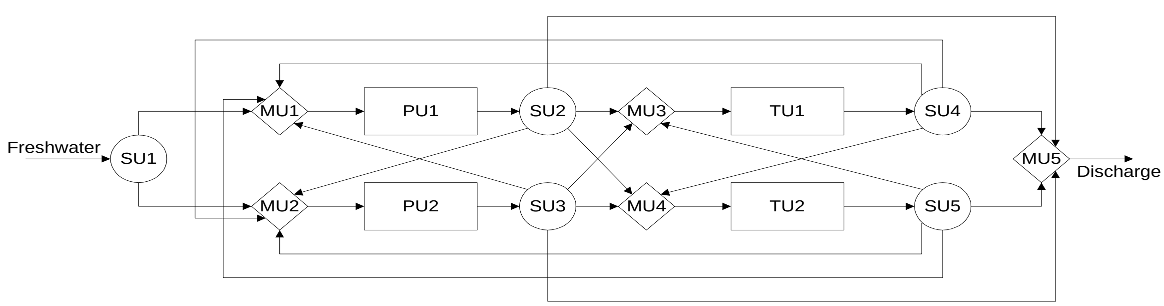

Fig. 3a Superstructure of integrated network with 2 Process units and 2 Treatment units

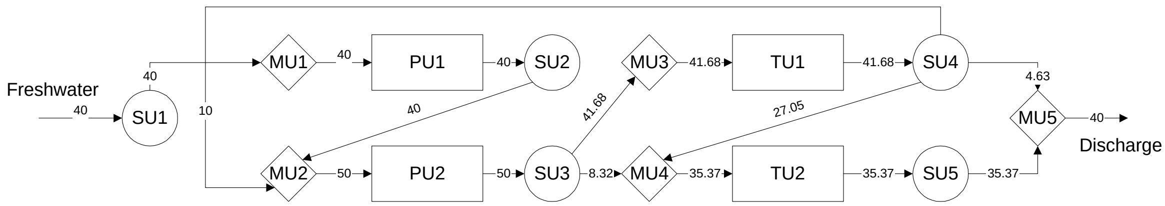

Fig. 3b Optimal solution for water network with 2 Process Units – 2 Treatment Units

One problem with the optimization of integrated water networks is that the model sizes for the integrated network synthesis problem are much larger compared to the sequential optimization problems. However, as will be shown, the proposed global optimization technique presented in this paper is able to find the global optimum in a reasonable amount of time.

3. Problem Statement

Given is an integrated water network that consists of a set of process units (PU) (e.g. scrubbers, liquid-liquid extraction units) that generate contaminants, treatment units (TU) (e.g. oil separators, centrifuges) that selectively remove them, and mixers (MU) and splitters (SU), with various possible interconnections between the units. The problem is then to synthesize an integrated network with these water using and water treating units in order to minimize the freshwater and wastewater flows, or more generally the total cost. In order to address this problem, we construct a superstructure, which is a generalization of the superstructure with two process units and two treatment units shown in Fig. 3a. Here, a freshwater source is present at the inlet of the network, from which freshwater is fed to the process units. These process units, in turn, are interconnected in all possible ways and also to the treatment units by making use of mixers and splitters. Similarly, the treatment units are also interconnected in all possible ways and with a final single stream that is discharged into the environment. There is also an option of bypassing wastewater generated in the process units directly to the discharge without any treatment.

For this synthesis problem the water flow demands of the process units are assumed to be fixed. For systems where the water using operations can take in a variable amount of water, the network modeling and optimization procedure remains the same. Upper bounds are often specified on the contaminant concentrations that are allowed in the inlet and outlet streams for each process unit. These are usually based on considerations of minimum mass transfer driving force, solubility of the contaminants, fouling and corrosion limitations. As for the treatment units, these remove a fraction of selected pollutants from an incoming wastewater stream, and this fraction is specified by a fixed removal ratio for each contaminant. These units may also have an inlet concentration restriction for the contaminants coming in. Wastewater treated in these units can be either discharged into the environment, such that the environmental limitations hold in the final discharge stream, or it can be recycled for use in the water using operations. As can be seen in Fig. 3a, each water using and treatment unit is preceded by a mixer, which merges freshwater, and/or the reuse flows coming out from the remaining operations. The flow coming out of each water using/treatment unit as well as the flow from the freshwater source is split into several streams and sent to various mixers in the network.

Following the above description of the superstructure of the integrated water network, the specific design problem can be stated as follows. We are given a set of water using and treatment units, a freshwater source (assumed to be devoid of any contaminants) to satisfy the demand in the water using processes, and also the costs associated with obtaining freshwater and treating wastewater. It is known that a certain number of contaminants are picked up in the water using processes, which are then removed in the treatment units. Mass balances in these units, as well as in the mixers and splitters, which help connecting the process and treatment units into a network, have to hold. Other constraints that have to be satisfied are that the contaminant composition of certain streams must not exceed specified values, and the contaminant concentrations have to be reduced to environmental limits before discharge. The aim of the design problem is to determine the flowrate and contaminant composition of each stream in the network such that the total annual cost of freshwater consumption and wastewater treatment is minimized.

The next step is to mathematically model the network. In the initial part of this work, we model the network as a continuous NLP problem. Later in the paper, we allow for selection of different technologies for the treatment operations, and hence binary variables are associated with each choice of a treatment technology and the problem is formulated with an MINLP model. Certain simplifying assumptions are made prior to modeling the system:

(i) The total flowrate of a stream is taken to be equal to that of pure water in that stream since the individual contaminant flows are negligible (ppm levels).

(ii) The cost is determined by the flows of freshwater and the flows inside the treatment units. The cost of pumping and cost of pipeline is neglected.

(iii) The network is operated under isothermal and isobaric conditions.

4. Model

There are two major ways to model the optimization problem. One of them is to use total flows and compositions of the streams in the material balance equations for each unit in the system. Alternatively, we can use individual flows of the components in a stream to formulate the mass balance equations. These mass balance equations for the multicomponent streams are the source of the non-convexities in the model. Non-convex bilinear terms are present in these equations and are responsible for giving rise to multiple local optima. Moreover, the failure of local NLP algorithms to find feasible points is often caused by numerical singularities, which arise when the flows in the bilinearities take values of zero (Quesada and Grossmann, 1995b). The assumptions made about the system are such that, on using the former model the mass balance equations for the mixer units contain the bilinearities, while in the latter model the non-linearities are present only in the equations for the splitter units. The model involving total flows and compositions contains fewer bilinearities (given that there are equal number of mixer and splitter units in the proposed superstructure) than the individual flows model, and can therefore be expected to be less difficult to solve than the other model. Another advantage of using the total flows and compositions representation is that the bounds of these variables are of the same order of magnitude, and so optimizing this model is expected to scale well numerically, whereas in the model involving individual flows and split fractions (these are unknown and present in the equations for the splitter units), the variable bounds differ significantly in magnitude and the optimization could run into numerical difficulties. Hence, the proposed optimization model is formulated using the total flows and compositions model as shown below.

Objective Function. A straightforward objective would be to minimize the sum of the freshwater intake into the system (*FW*) and the total flow of wastewater being treated inside the treatment units (F^i , i is the outlet stream for a treatment unit denoted by *t*, $i \in t_{out}$). For simplicity equal weights are assigned to the flows, although relative weights can easily be used.

$$\min \quad \Phi \quad = \quad FW + \sum_{\substack{t \in TU \\ i \in t_{out}}} F^i \tag{1a}$$

More often, the optimization problem is solved using more complex cost functions in the objective function:

$$\min \quad \Phi \quad = \quad HC_{FW}FW + AR\sum_{\substack{t\in TU \\ i\in t_{out}}} IC^t\left(F^i\right)^{\alpha} + H\sum_{\substack{t\in TU \\ i\in t_{out}}} OC^t F^i \tag{1b}$$

where H = Hours of operation of plant per annum (hrs)

C_{FW} = Cost of freshwater ($/ ton)

FW = Freshwater intake into the system (ton/ hr)

AR = Annualized factor for investment on treatment units

$IC^t(F^i)^{\alpha}$ = Investment cost of a treatment unit t ($)

$OC^t F^i$ = Operating cost of a treatment unit t ($/ hr)

α = Cost function exponent ($0 < \alpha \leq 1$)

All streams in the superstructure are labeled as F^i (i = 1,2, … ,N_{st}), where N_{st} is the total number of streams in the superstructure.

Mixer Units. In Fig. 4, a mixer $m \in$ MU is shown consisting of a set of inlet streams i that are specified in the index set m_{in}, and an outlet stream $k \in m_{out}$. The overall material balance for the mixer m is given by eq (2) and the mass balances for each contaminant j in that mixer are given in eq (3).

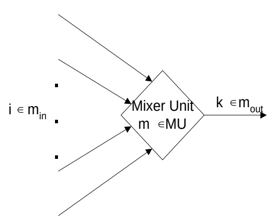

Fig. 4 Mixer Unit

$$F^k = \sum_{i\in m_{in}} F^i \quad \forall m \in MU \;, \forall k \in m_{out} \tag{2}$$

$$F^k C_j^k = \sum_{i\in m_{in}} F^i C_j^i \quad \forall j, \forall m \in MU, \forall k \in m_{out} \tag{3}$$

Here F^i is the total flow of stream i (in ton/ hr) and C_j^i is the contaminant concentration (in ppm) in stream i. The individual contaminant balance equations contain the non-convex bilinear terms.

Splitter Units. As shown in Fig. 5, a splitter $s \in$ SU consists of an inlet stream $k \in$ s_{in} and a set of outlet streams i specified in the index set s_{out}. The contaminant composition in the streams leaving the splitter is equal to the composition in the inlet stream. The following linear equations model the splitter s:

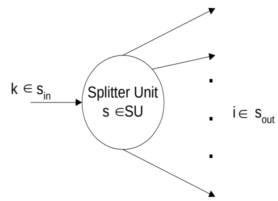

Fig. 5 Splitter Unit

$$F^k = \sum_{i \in s_{out}} F^i \quad \forall s \in SU, \forall k \in s_{in} \tag{4}$$

$$C_j^i = C_j^k \quad \forall j,\ \forall s \in SU, \forall i \in s_{out}, \forall k \in s_{in} \tag{5}$$

Process Units. A process unit $p \in$ PU consists of an inlet stream $i \in$ p_{in} and an outlet stream $k \in$ p_{out} as shown in Fig. 6. The contaminant load inside the process unit p is assumed to be constant for each pollutant j and is given by L_j^p (in kg / hr). The process unit is described by the following equations:

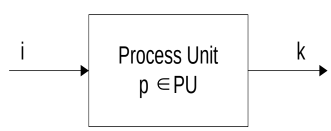

Fig. 6 Process Unit

$$F^k = F^i = P^p \quad \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out} \tag{6}$$

where P^p is a constant (in ton / hr) for each process unit p.

$$P^p C_j^i + L_j^p \times 10^3 = P^p C_j^k \quad \forall j, \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out} \tag{7}$$

In eq (7), P^p is in ton/hr, L_j^p is in kg/hr and C_j^i is in ppm and so a multiplication factor of 10^3 is required to make this equation dimensionally correct. When variable flows are allowed through the process units, the change is in eq (7) where P^p is replaced by F^k which is a variable.

Treatment Units. As shown in Fig. 7, a treatment unit $t \in$ TU has an inlet stream $k \in$ t_{in} and an outlet stream $i \in$ t_{out}. The individual contaminant flows in the outlet stream i can be expressed as a linear function of the individual flows in the inlet stream k in terms of the coefficients β_j^t, where β_j^t = 1 – {(Removal ratio for contaminant j in unit t (in %)) / 100 }. Since the inlet and outlet flows for a treatment unit are equal (eq (8)), the mass balance equation for each contaminant *j* inside the treatment unit *t* becomes linear and is shown in eq (9).

Fig. 7 Treatment Unit

$$F^k = F^i \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in} \tag{8}$$

$$C_j^i = \beta_j^t C_j^k \quad \forall j, \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in} \tag{9}$$

All the flows (F^i), and contaminant concentrations (C_j^i) in the system are non-negative.

Feasibility analysis of the network

For networks with fixed contaminant loads and fixed flow demands in the process units and constant removal ratios in the treatment units, the feasibility of the network can be determined without solving the NLP by analyzing the values of these parameters and the given environmental discharge limit. Here, the feasibility issue comes into play only at the wastewater discharge point into the environment, where the environmental discharge limits on the contaminant concentrations must hold. The feasibility criteria is derived based on the extreme case of using only freshwater to fulfill the demand of each process unit (without any reuse/ recycle) and then merging the wastewater streams into a single stream which is then treated sequentially in all the available treatment units without any bypass.

Let us consider a system with have a system with n_p process units and n_t treatment units and assume the environmental discharge limit for a contaminant *j* to be δ_j (in ppm). The constraint that has to be satisfied for network feasibility is:

$$\left(\beta_j^1\right)\left(\beta_j^2\right)\ldots\left(\beta_j^{nt}\right)\frac{\sum_{p=1}^{np} L_j^p \times 10^3}{\sum_{p=1}^{np} P^p} \quad \leq \quad \delta_j \qquad \forall j \tag{F1}$$

For the case, when there is also a restriction on the amount of contaminant flow to be discharged into the environment, the following inequality must also hold:

$$\left(\beta_j^1\right)\left(\beta_j^2\right)\ldots\left(\beta_j^{nt}\right)\sum_{p=1}^{np} L_j^p \quad \leq \quad \zeta_j \qquad \forall j \tag{F2}$$

where ζ_j is the maximum flow of pollutant j (in kg/hr) allowed in the discharge.

If any equation in the set of equations (F1) and (F2) is not satisfied, then no structure embedded in the superstructure would be feasible for the integrated water network, and more treatment units would be required to be added to the superstructure to be able to generate a feasible design.

5. Relaxation of the non-linear model

To solve the non-convex NLP optimization problem given by eqs (1) – (9), we propose a deterministic global optimization technique. These techniques are guaranteed to converge to the global optimum, given a specified tolerance for the gap between the NLP and its convex relaxation. Most of the deterministic global optimization techniques involve some form of a spatial branch and bound procedure. At every node of such a branch and bound tree, lower bounds on the value of the objective function (for a minimization problem) are obtained by solving a convex relaxation of the original NLP problem. A Linear Programming (LP) relaxation of the given non-linear model can be constructed by replacing the bilinear terms $F^i C_j^i$ in eq (3) with f_j^i (eq (10)), and then introducing the following linear inequalities (eq (11)) into the model:

$$f_j^k = \sum_{i \in m_{in}} f_j^i \qquad \forall j, \forall m \in MU, \forall k \in m_{out} \tag{10}$$

$$
\begin{aligned}
&f_j^i \geq F^{iL} C_j^i + C_j^{iL} F^i - F^{iL} C_j^{iL} \\
&f_j^i \geq F^{iU} C_j^i + C_j^{iU} F^i - F^{iU} C_j^{iU} \\
&f_j^i \leq F^{iL} C_j^i + C_j^{iU} F^i - F^{iL} C_j^{iU} \\
&f_j^i \leq F^{iU} C_j^i + C_j^{iL} F^i - F^{iU} C_j^{iL} \qquad \forall j, \forall m \in MU, \forall i \in m_{in}, \forall i \in m_{out}
\end{aligned} \tag{11}
$$

The constraints in eq (11) correspond to the convex and concave envelopes of the bilinear terms over the bounds on the total flows $F^{iL} \leq F^i \leq F^{iU}$ and the contaminant compositions $C_j^{iL} \leq C_j^i \leq C_j^{iU}$ (McCormick, 1976). These can be derived based on the reformulation and linearization technique for bilinear programming models proposed by Sherali and Alameddine (1992). Further, to eliminate the non-linearity in the objective function, we replace each concave cost function term $\left(F^i\right)^\alpha$, present in the original non-linear model, by $\overline{F}^i$ in the LP relaxation and bound this function by its underestimator $\left(\hat{F}^i\right)$, which is the secant line for the concave function $\left(F^i\right)^\alpha$ between the bounds F^{iL} and F^{iU}. Due to this transformation, the relaxed objective function becomes linear in nature and is given by:

$$
\Phi_{\text{relax}} = HC_{FW} FW + AR \sum_{\substack{t \in TU \\ i \in t_{out}}} IC^t \left(\overline{F}^i\right) + H \sum_{\substack{t \in TU \\ i \in t_{out}}} OC^t F^i \tag{12}
$$

where the underestimation of the concave term is given by,

$$
\overline{F}^i \geq \hat{F}^i = \left(F^{iL}\right)^\alpha + \left(\frac{\left(F^{iU}\right)^\alpha - \left(F^{iL}\right)^\alpha}{F^{iU} - F^{iL}}\right)\left(F^i - F^{iL}\right) \tag{13}
$$

The solution of the Linear Programming (LP) relaxation may, however, yield weak valid lower bounds, which slows down the convergence of the branch and bound algorithm. In order to strengthen the lower bounds obtained from the relaxation, we partition the original rectangular domain D = $[F^L, F^U] \times [C^L, C^U]$ of each bilinear term *FC* into rectangular strips (D_1, D_2, …, D_N), based on N+1 intermediate points for the flows, $F^L = F_1$, F_2, …, $F_{N+1} = F^U$, and use piecewise linear under- and over-estimators for the bilinear terms over each partition (Fig. 8) (see Bergamini et al., 2004). These partitions are identical for each bilinear term. This partitioning is then also used to construct piecewise underestimators for the concave functions $\left(F^{i}\right)^{\alpha}$ over each partition as illustrated in Fig. 9.

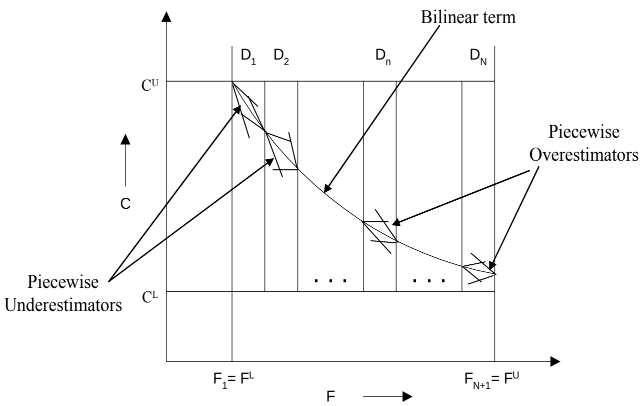

Fig. 8 Construction of Piecewise estimators for bilinear terms

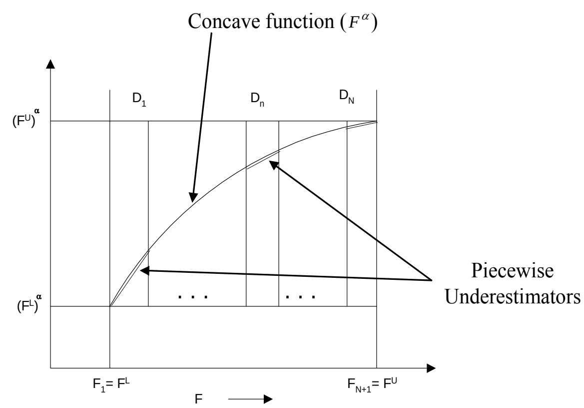

Fig. 9 Piecewise underestimators for concave cost functions

We formulate the partitioning of the domain D and the construction of the piecewise estimators over each interval $D_n = [F_n, F_{n+1}] \times [C^L, C^U]$ through the following disjunction:

$$\bigvee_{n=1\ldots N}\left[\begin{array}{c} W_n \\ f^{u} = \max\left\{FC^{L} + F_n C - F_n C^{L}\ ,\ FC^{U} + F_{n+1}C - F_{n+1}C^{U}\right\} \\ f^{o} = \min\left\{FC^{L} + F_{n+1} C - F_{n+1} C^{L}\ ,\ FC^{U} + F_{n}C - F_{n}C^{U}\right\} \\ \hat{F} = \left(F_n\right)^{\alpha} + \left(\dfrac{\left(F_{n+1}\right)^{\alpha} - \left(F_n\right)^{\alpha}}{F_{n+1} - F_n}\right)\left(F - F_n\right) \quad \forall t \in TU \\ F_n \le F \le F_{n+1}\ ,\ C^{L} \le C \le C^{U} \end{array}\right]$$
$$W_n \in \{true,\ false\}$$

where, f^{u} and f^{o} denote the piecewise under- and over-estimators respectively, for the bilinear term *FC*, and $\hat{F}$ denotes the underestimator for the concave term F^{α}, over the region D_n. If the boolean variable W_n holds true, then all the constraints in the n[th] disjunct are enforced, while the constraints in all the other disjuncts are neglected. So only those piecewise estimators that are constructed over D_n would exist.

The underestimating problem is then converted into an MILP with the following formulation, which is based on the convex hull reformulation of the disjunctions (Balas, 1985).

$$
\begin{aligned}
&F = \pi_1 + \pi_2 + \ldots + \pi_N \; ; \quad C = \chi_1 + \chi_2 + \ldots + \chi_N \\
&FC \geq \sum_{n=1}^{N} \max\{\pi_n C^L + F_n \chi_n - F_n C^L \lambda_n \, , \pi_n C^U + F_{n+1}\chi_n - F_{n+1} C^U \lambda_n\} \\
&FC \leq \sum_{n=1}^{N} \min\{\pi_n C^L + F_{n+1} \chi_n - F_{n+1} C^L \lambda_n \, , \pi_n C^U + F_n \chi_n - F_n C^U \lambda_n\} \\
&(F)^\alpha \geq \sum_{n=1}^{N} \left((F_n)^\alpha \lambda_n + \left(\frac{(F_{n+1})^\alpha - (F_n)^\alpha}{F_{n+1} - F_n} \right) (\pi_n - F_n \lambda_n) \right) \qquad \forall t \in TU \\
&F_n \lambda_n \leq \pi_n \leq F_{n+1} \lambda_n \; ; \; C^L \lambda_n \leq \chi_n \leq C^U \lambda_n \qquad n = 1, \ldots, N \\
&\sum_{n=1}^{N} \lambda_n = 1 \; ; \; \lambda_n \in \{0,1\}
\end{aligned}
\tag{14}
$$

These piecewise estimators match the values of the original bilinear and concave terms at the bounds of each sub-region. Further, it is to be noted here, that the partitioning is done in one unique dimension (only on the flows and not on the compositions) in order to avoid increasing the number of binary and continuous variables in the formulation. Partitioning carried out on the compositions was not found to be computationally effective in tightening the bounds.

Non-redundant bound strengthening cuts

Linear constraints that correspond to the contaminant flow balances for the overall system (eq (15)) are incorporated as cuts into the relaxed model. These cuts are redundant in the original NLP,

$$\sum_{p \in PU} L_j^p \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \left(1 - \beta_j^t\right) f_j^k + f_j^{out} \quad \forall j \tag{15}$$

where f_j^{out} is the flow of contaminant j in the outlet stream to the environment.

It was found that these linear equalities serve as deep cuts in the relaxation, improving substantially the quality of the lower bounds, and thereby helping to reduce the computational time for solving the lower bounding problem at every node in the tree. Qualitatively, the reason for the usefulness of these cuts is that the relaxation of the mass balances in the mixers causes the violation of the overall mass balance of the individual contaminants and the addition of these cuts remedies this problem.

Logic Cuts

Based on the physical nature of the system, we derive some logic integer constraints, which help to reduce the time for solving the relaxation. Consider two flow variables F^a and F^b, which are related by an equality constraint $F^a = F^b$ and have common lower and upper bounds $F^{aL} = F^{bL}$ and $F^{aU} = F^{bU}$. It is valid to state that if the nth term of the disjunctions pertaining to the construction of the piecewise estimators holds true for the variable F^a, i.e. W_n^a is true, then the nth term of the disjunctions holds true for F^b as well, i.e. W_n^b is also true. Qualitatively, this means that if we have two streams that are supposed to have equal flow rates, and if one of them lies in a certain interval, the other flow also has to lie in the same interval since the partitioning for the flows is identical. In terms of the boolean variables W_n^a and W_n^b, the above statement can be written as $W_n^a \Leftrightarrow W_n^b \quad (n = 1 \ldots N)$. This logic proposition transforms into the following integer constraint:

$$\lambda_n^a = \lambda_n^b \qquad n = 1 \ldots N \tag{16}$$

The logic proposition is graphically depicted in Fig. 10.

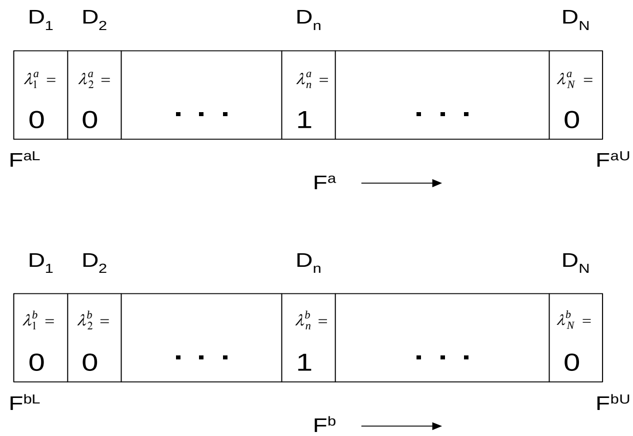

Fig. 10 Diagrammatic representation of a logic cut

Fig. 10 shows the partitioning of two flows which are equal to each other in the model and lie between the same bounds. Both flows are divided into N equal intervals. The logic integer cut just means that, if for one of the flows, the piecewise estimators are constructed over the domain D_n, then the piecewise estimators are constructed over the same domain for the other flow also. So the integer variable λ_n corresponding to domain D_n has a value equal to 1 for both the flows.

The relaxation of the original NLP comprises the equations (2), (4)-(10), (12), (14), (15) and the relevant integer cuts (derived for only certain flow variables, eq (16)) and is shown below as model (CR).

$$\min \Phi_{\text{relax}} \quad = \quad HC_{FW}FW + AR\sum_{\substack{t\in TU \\ i\in t_{out}}} IC^t\left(\overline{F}^{\,i}\right) + H\sum_{\substack{t\in TU \\ i\in t_{out}}} OC^t F^i$$

$$
\begin{aligned}
s.t.\quad & F^{k} = \sum_{i\in m_{in}} F^{i} \quad \forall m \in MU, \forall k \in m_{out} \\
& f_j^{k} = \sum_{i\in m_{in}} f_j^{i} \quad \forall j, \forall m \in MU, \forall k \in m_{out} \\
& F^{k} = \sum_{i\in s_{out}} F^{i} \quad \forall s \in SU, \forall k \in s_{in} \\
& C_j^{i} = C_j^{k} \quad \forall j, \ \forall s \in SU, \forall i \in s_{out}, \forall k \in s_{in} \\
& F^{k} = F^{i} = P^{p} \quad \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out} \\
& P^{p} C_j^{i} + L_j^{p} \times 10^{3} = P^{p} C_j^{k} \quad \forall j, \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out} \\
& F^{k} = F^{i} \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in} \\
& C_j^{i} = \beta_j^{t} C_j^{k} \quad \forall j, \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in} \\
& F = \pi_1 + \pi_2 + \dots + \pi_N \ ; \quad C = \chi_1 + \chi_2 + \dots + \chi_N \\
& FC \geq \sum_{n=1}^{N} \max\{ \pi_n C^{L} + F_n \chi_n - F_n C^{L} \lambda_n \ , \pi_n C^{U} + F_{n+1}\chi_n - F_{n+1} C^{U} \lambda_n \} \\
& FC \leq \sum_{n=1}^{N} \min\{ \pi_n C^{L} + F_{n+1} \chi_n - F_{n+1} C^{L} \lambda_n \ , \pi_n C^{U} + F_n \chi_n - F_n C^{U} \lambda_n \} \\
& (F)^{\alpha} \geq \sum_{n=1}^{N} \left((F_n)^{\alpha} \lambda_n + \left(\frac{(F_{n+1})^{\alpha} - (F_n)^{\alpha}}{F_{n+1} - F_n} \right) (\pi_n - F_n \lambda_n) \right) \qquad \forall t \in TU \\
& F_n \lambda_n \leq \pi_n \leq F_{n+1} \lambda_n \ ; \ C^{L} \lambda_n \leq \chi_n \leq C^{U} \lambda_n \qquad n = 1, \dots, N \\
& \sum_{n=1}^{N} \lambda_n = 1 \ ; \ \lambda_n \in \{0,1\} \\
& \sum_{p\in PU} L_j^{p} \times 10^{3} = \sum_{\substack{t\in TU \\ k \in t_{in}}} \left(1 - \beta_j^{t}\right) f_j^{k} + f_j^{out} \quad \forall j \\
& \lambda_n^{a} = \lambda_n^{b} \quad \forall n, \forall a, b \quad s.t. \quad F^{a} = F^{b} \, and \ \ F^{aL} = F^{bL} \, and \ \ F^{aU} = F^{bU}
\end{aligned} \qquad \text{(CR)}
$$

The solution of this MILP provides a tight lower bound on the solution of the non-convex NLP problem as compared to the LP relaxation of NLP. Due to these tightened bounds, making use of the MILP relaxation in the global optimization algorithm accelerates the convergence of the algorithm, even though it is cheaper to solve an LP relaxation at each node of the branch and bound tree vis-à-vis solving the MILP relaxation. The next section describes the use of this MILP within a global optimization algorithm.

6. Global optimization algorithm for non-convex NLP problems

The outline of the proposed global optimization algorithm is as follows:

Step 0. Preprocessing The bounds on the variables in the system (F^i and C_j^i) are determined by physical inspection of the superstructure and using the numerical data given for the process and treatment units. Based on the data for a specific problem, some variables can be further bounded or fixed to certain values. The set of variables appearing in the non-convex terms are known as complicating variables. The bounds of these variables are important because they are a part of the estimator equations in the relaxation, and hence affect the tightness of the lower bound obtained by solving the relaxation. In this step, the original non-convex NLP is locally optimized to obtain an initial overall upper bound (OUB) on the objective function.

Step 1. Bound Contraction Procedure (BCP) (Optional) The upper and lower bounds of the flow variables appearing in the bilinear terms are contracted using a simplified version of the method by Zamora and Grossmann (1999),

$$\min/\max \; F^i$$

$$\text{s.t.} \quad HC_{FW} FW + AR \sum_{\substack{t \in TU \\ i \in t_{out}}} IC^t\left(\hat{F}^i\right) + H \sum_{\substack{t \in TU \\ i \in t_{out}}} OC^t F^i \leq OUB \tag{17}$$

eqs (2), (4) – (11), (13), (15)

If we have a linear objective function in the original non-linear model, eqn (17) is replaced by $FW + \sum_{\substack{t \in TU \\ i \in t_{out}}} F^i \leq OUB$. This set of minimization and maximization problems, which are all LP's, have unique solutions and help in eliminating parts of the original feasible region where the global optimum does not lie. This step can be performed at every node of the Branch and Bound tree so as to reduce the search space, and to tighten the under- and over-estimators for the non-convex terms in the relaxation, so that the search is accelerated. The bound contraction sub-problem is illustrated in Fig. 11.

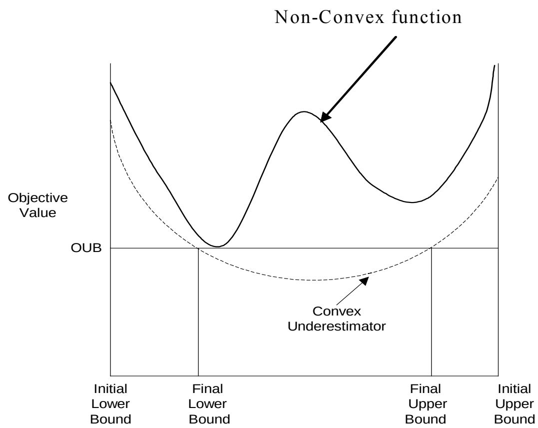

Fig. 11 Bound Contraction Subproblem

The figure shows that the constraint involving the overall upper bound chops off parts of the feasible region where the relaxed objective function takes values greater than the OUB.

Step 2. Lower Bounding MILP problem The MILP (CR) is solved over a given subregion minimizing the relaxed objective function to obtain lower bounds (LB) on the global optimum at every node of the tree. If the solution of the lower bounding problem is found to be infeasible, the node is fathomed from the tree. Note that the original non-convex NLP is infeasible if its convex relaxation is found to be infeasible at the root node of the branch and bound tree.

Step 3. Upper Bound (UB) The solution of the relaxed MILP problem is used as a starting point to solve the original non-convex NLP to obtain an upper bound, and the OUB is updated if there is an improvement.

Step 4. Convergence A node can be discarded from the tree if the lower bound at that node is greater than the current OUB, or it is within a tolerance ε of the OUB. For the ε convergence criteria, nodes at which the relaxation gap (gap_{node}) is less than ε, are fathomed. The relaxation gap is defined as:

$$gap_{node} = \begin{cases} \left| \dfrac{OUB - LB_{node}}{OUB} \right| & if\ OUB \neq 0 \\ -LB_{node} & if\ OUB = 0 \end{cases}$$

The search is stopped when no open nodes are left in the tree.

<u>*Step 5. Spatial Branch and Bound*</u> All active regions of the original domain (for which the relaxation gap between the OUB and the LB is greater than the specified tolerance) are further partitioned into disjoint sub-regions, according to some rules, and we repeat steps 1 to 4 for each of these regions. The estimator equations are updated in each partition, and so we obtain tighter lower bounds over each of the sub-regions. In a tree representation, this division of the original domain into two sub-regions corresponds to branching down a parent node to create two child nodes. In this work, certain heuristics are followed as branching rules. The branching is performed on the flow variables. From the solution of the lower bounding problem, we compute the sum of the absolute gap between the non-convex term and its convex underestimator $\left(\sum_j \left| F^i C_j^i - f_j^i \right| \right)$ over all contaminants for each flow, and the flow for which the value of this sum is maximum, is chosen as the branching variable. Finally, we select the mid-point of the variable bounds as the branching point (bisection rule). A depth first strategy is used to traverse the nodes of the tree. Theoretically, the spatial branch and bound is an infinite process since the branching is done on the continuous variables, but terminates in a finite number of nodes for $\varepsilon-$ convergence.

Remarks

1. The bound contraction is not performed on the contaminant concentration variables in this work, saving some computational effort, although it can easily be done in the same way as for the flow variables.

2. If the bound contraction sub-problem is found to be infeasible, then either the feasible region of the convex relaxation is empty, or the relaxed objective function cannot take a value below the existing OUB.
3. In using piecewise estimators to approximate the non-convex functions at any node of the branch and bound tree, if the region between the bounds of the variables is not partitioned into equal intervals for the construction of the piecewise estimators, or the bisection rule is not followed for the branching, there can be non-increasing lower bounds for some nodes down the tree. It should be stressed that though this affects the efficiency of the search, it does not impact the rigor of the search and the global optimum is never cut off since the lower bounds obtained are always valid. This problem can be remedied by using all the piecewise estimator equations at a given node's parent node in addition to the estimators constructed at the current node for solving the convex relaxation of the original NLP.
4. Unless the estimator information from the parent node of a given node is also used in solving the lower bounding problem at the node, performing the bound contraction operation for all the flow variables at every node of the spatial branch and bound tree can also lead to the same problem of non-increasing lower bounds down the tree. This problem can be avoided in the following ways:
   - (i) Solve the bound contraction problem only at the root node to get contracted bounds on the variables, and at no other node in the tree.
   - (ii) At a given node, after the bound contraction has been performed on a certain variable *F*, keep as the partitioning points, the newly created lower bound

$\left(F_{new}^{L}\right)$, the new upper bound $\left(F_{new}^{U}\right)$, and all those partitions of the node's parent node, which lie between $\left(F_{new}^{L}\right)$ and $\left(F_{new}^{U}\right)$.

(iii) At a given node, perform bound contraction on only those variables which were not ε_x - close to any of the partitions F_2, … F_N in the solution of the relaxation (MILP) at its parent node. Let us assume that $F_{relax}^{parent,v}$ is the optimal value of a variable *F* obtained by solving the lower bounding problem at the parent node of a node *v*, and we are given a positive parameter ε_x, then the term ε_x - close to any of F_2, … , F_N means that one of the following constraints holds:

$$F_{relax}^{parent,v} \le \begin{matrix} F_n(1+\varepsilon_x) & if\ F_n \neq 0 \\ \varepsilon_x & if\ F_n = 0 \end{matrix} \qquad n = 2, \ldots, N$$

or

$$F_{relax}^{parent,v} \ge F_n(1-\varepsilon_x) \quad if\ F_n \neq 0 \qquad n = 2, \ldots, N$$

For such a variable *F*, which meets one of the above criteria, bound contraction may not be carried out at the node *v*. This method reduces the chances of the occurrence of the non-increasing lower bound problem, but does not guarantee its elimination altogether.

5. To reduce the computational expense of the lower bounding problem (which is the most expensive step of the branch and bound scheme), we implement a constraint in the lower bounding problem that cuts off nodes directly from the MILP branch and bound tree, where the relaxed objective function is greater than the OUB.

7. Examples

The proposed method has been applied to the optimization of several integrated water networks. All the examples were solved with GAMS (Brooke et al., 1998) on an Intel 2.5 GHz machine with 512 MB memory. GAMS/CONOPT3 was used to solve the NLP problems, GAMS/CPLEX 9.0 was used for the LP and MILP problems, and GAMS/DICOPT++ was applied for solving the MINLP problems. In calculating the total computational time for solving a problem, the NLP solution times in the global optimization algorithm were found to be insignificant as they were of the order of a hundredth of a second. The computational expense of the proposed algorithm was compared with that of using GAMS/BARON 7.2 (Sahinidis, 1996), a general purpose software for global optimization. In all the cases, BARON was supplied with original bounds on the variables obtained from the pre-processing step. The tolerance selected for the optimization was $\varepsilon = 0.01$. Further, we divide the space between the bounds of the complicating variables into equal intervals, while constructing the lower bounding problems in all the examples. The number of intervals is chosen heuristically. The problem sizes of these examples are given in Table 9a and the numerical results for all these problems are summarized in Table 9b.

<u>Example 1</u> As a first example, we consider a network whose superstructure is shown in Fig. 3a. It is a 2 process unit and 2 treatment unit system involving two contaminants A and B, for which process unit and treatment unit data are given in Table 1 and in Table 2, respectively.

Table 1. Process Unit data for Example 1

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)		Maximum Inlet Concentration (ppm)	
		A	B	A	B
PU1	40	1	1.5	0	0
PU2	50	1	1	50	50

Table 2. Treatment Unit data for Example 1

Unit	Removal ratio (%) A	B
TU1	95	0
TU2	0	95

The environmental discharge limit for both the contaminants (A and B) is taken to be 10 ppm. The objective in this example is to minimize the freshwater consumption and wastewater treated in the network (eq (1a)). While applying the proposed algorithm for solving this problem, the bound contraction procedure (step 2, Section 6) is employed only at the root node of the branch and bound tree. Fig. 3b shows the optimal network structure with an objective value of 117.05 ton/ hr.

Example 2 The superstructure for a 3 process unit and 3 treatment unit integrated network is optimized with the data given in Tables 3 and 4 in this example.

Table 3. Process Unit data for Example 2

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr) A	B	Maximum Inlet Concentration (ppm) A	B
PU1	40	1	1.5	0	0
PU2	50	1	1	50	50
PU3	60	1	1	50	50

Table 4. Treatment Unit data for Example 2

Unit	Removal ratio (%) A	B	IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
TU1	95	0	16800	1	0.7
TU2	80	90	24000	0.033	0.7
TU3	0	95	12600	0.0067	0.7

Again, there are two contaminants A and B in the system, and their concentrations in the wastewater have to be reduced to 10 ppm before the effluent stream is discharged into the environment. As opposed to example 1, the objective function here involves the cost of freshwater and the cost of treatment units (eq (1b)). The freshwater cost is assumed to be $1 / ton, the annualized factor for investment on the treatment units is taken to be 0.1, and the total time of operation of the plant in a year is taken as 8000 hours. The superstructure for this example network and its optimal structure with a cost of $ 381,751.35 / year are shown in Fig. 12 and Fig. 13, respectively. It can be seen in Fig. 13 that only one of the treatment units (TU2) is present in the optimal network structure, while the other treatment units (TU1 and TU3) are discarded by the optimization procedure. Note that the treatment unit TU2 removes both pollutants A and B, while the other two treatment units, each remove only one of the contaminants although with a higher removal efficiency. Hence, it is economically more viable to have one unit that is more expensive, but removes all contaminants with a lower efficiency, rather than two separate units that are cheaper but just remove only selected contaminants with a higher efficiency.

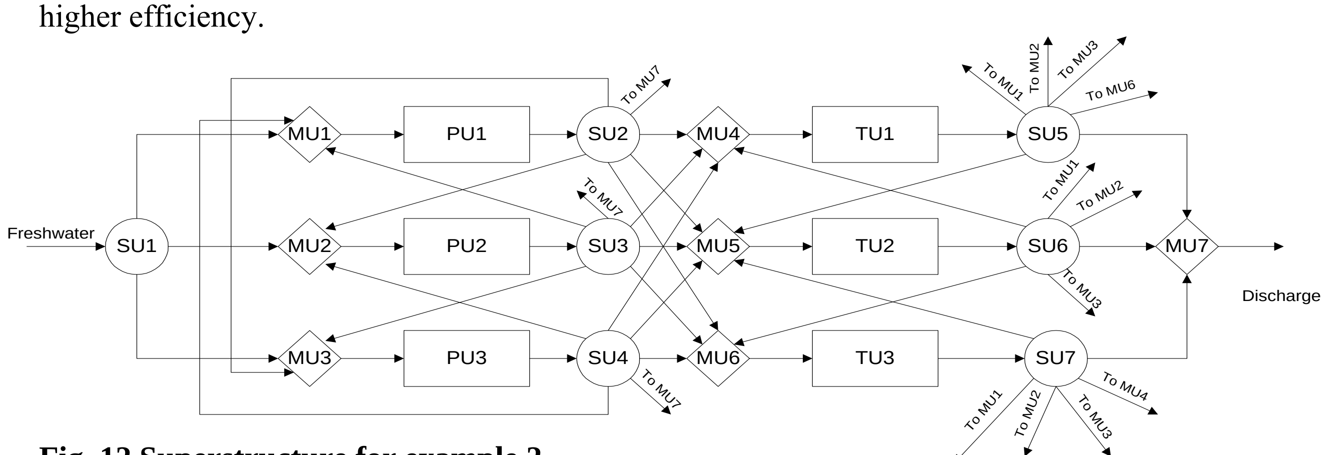

Fig .12 Superstructure for example 2

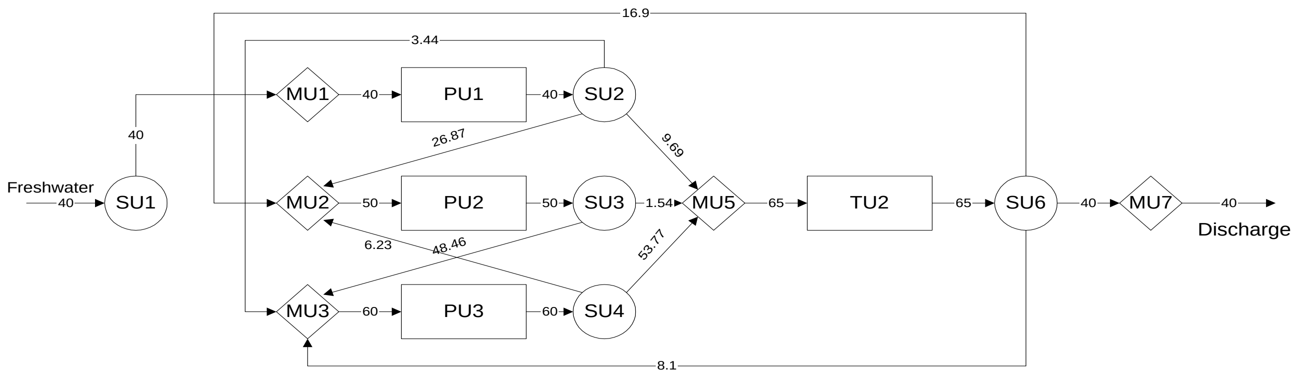

Fig. 13 Optimal network structure for example 2

A graphical illustration of the proposed spatial branch and bound algorithm for this example is presented in Fig. 14 where it can be seen that only 3 nodes are required to solve this problem.

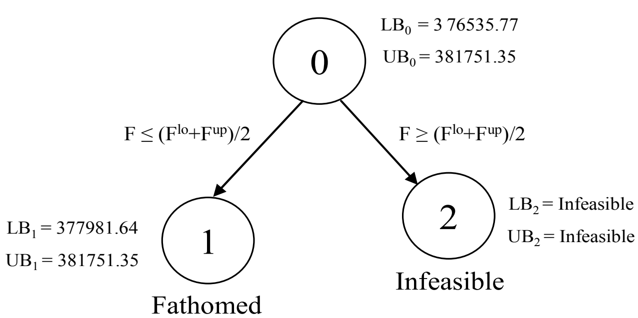

Fig. 14 Spatial branch and bound tree : Example 2

<u>Example 3</u> The third example involves optimizing a system with four process units and two treatment units. As in example 2, the environmental limit for the concentrations of the contaminants A and B is 10 ppm. A cost function is minimized in this example, with the cost of freshwater being \$ 1/ ton, the annualized factor for investment taken to be 0.1 and the other data taken from Tables 5 and 6. The plant is run for 8000 hrs/ year. Fig. 15 and Fig. 16 show the superstructure and the optimal design of the network, respectively. The globally optimal design yields a cost of \$ 874,057.37 / year, which is significantly lower than the cost of \$ 948,749.07 / year that is obtained by locally optimizing the network using the NLP solver CONOPT.

Table 5. Process Unit data for Example 3

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)		Maximum Inlet Concentration (ppm)	
		A	B	A	B
PU1	40	1	1.5	0	0
PU2	50	1	1	50	50
PU3	60	1	1	50	50
PU4	70	2	2	50	50

Table 6. Treatment Unit data for Example 3

Unit	Removal ratio (%)		IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
	A	B			
TU1	95	0	16800	1	0.7
TU2	0	90	12600	0.0067	0.7

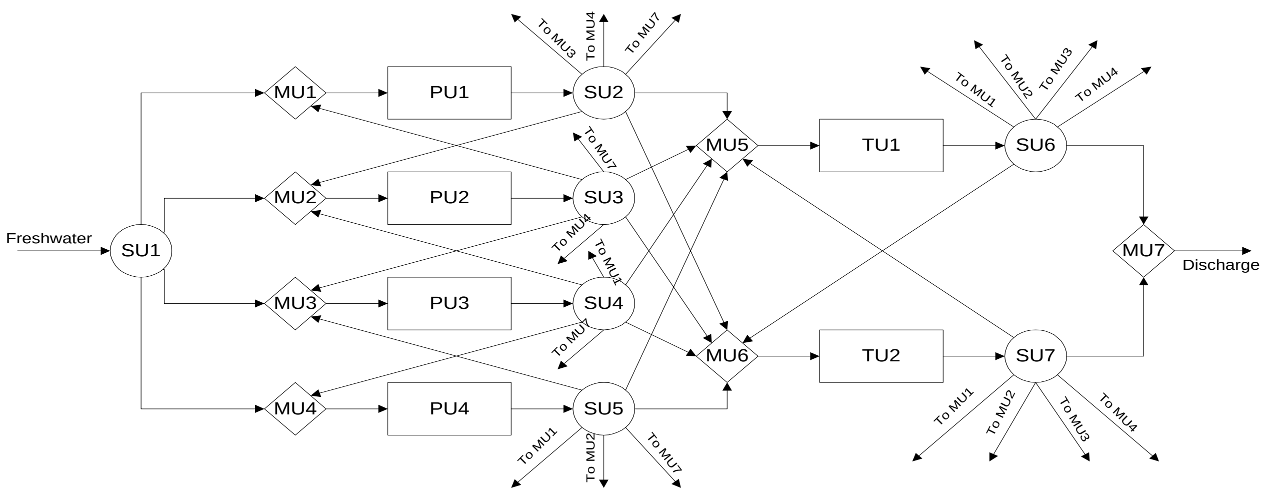

Fig. 15 Superstructure for example 3

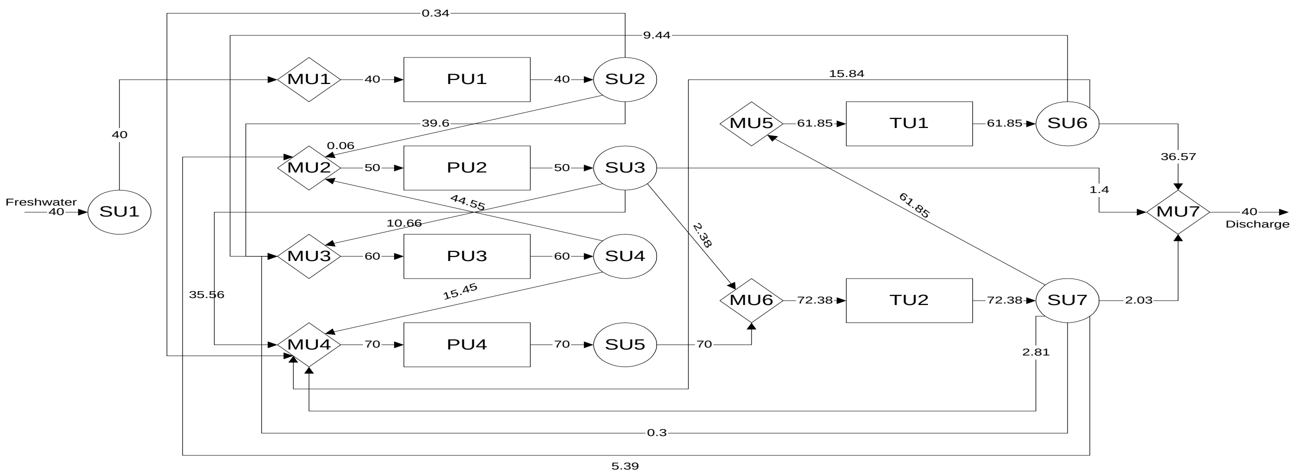

Fig. 16 Optimal solution of example 3

In Fig. 16 we can see that there are three streams whose flows are quite small. The stream that goes from splitter SU2 to the mixer MU4 has a flowrate of 0.34 ton/ hr, the one from splitter SU7 to mixer MU3 has a flow of 0.3 ton/ hr and the flow in the stream going from splitter SU2 to mixer MU2 is only 0.06 ton/ hr. The flows in the specified streams were fixed to zero and the superstructure optimization was carried out. It was found that there was no change in the objective function value ($ 874,057.37 / year) indicating that the global optimum for the network is not unique.

Example 4 As a final example, a large system with five process units and three treatment units is optimized. This system involves three contaminants (A, B and C) as compared to the two contaminant systems optimized earlier. The concentration of the pollutants in the discharge stream to the environment is constrained not to exceed 10 ppm. The superstructure (shown in Fig. 17) is optimized based on cost functions with data taken from Tables 7 and 8. The cost of freshwater, annualized factor for investment and hours of operation of the plant in a year that are used in the optimization were the same as in example 3. The optimal solution for the network is shown in Fig. 18. The cost of this design, $ 1,033,810.95 / year, is also substantially lower than the cost that is obtained with the local NLP solver CONOPT ($ 1,121,848.76 / year).

Table 7. Process Unit data for Example 4

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)			Maximum Inlet Concentration (ppm)		
		A	B	C	A	B	C
PU1	40	1	1.5	1	0	0	0
PU2	50	1	1	1	50	50	50
PU3	60	1	1	1	50	50	50
PU4	70	2	2	2	50	50	50
PU5	80	1	1	0	25	25	25

Table 8. Treatment Unit data for Example 4

Unit	Removal ratio (%)			IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
	A	B	C			
TU1	95	0	0	16800	1	0.7
TU2	0	0	95	9500	0.04	0.7
TU3	0	95	0	12600	0.0067	0.7

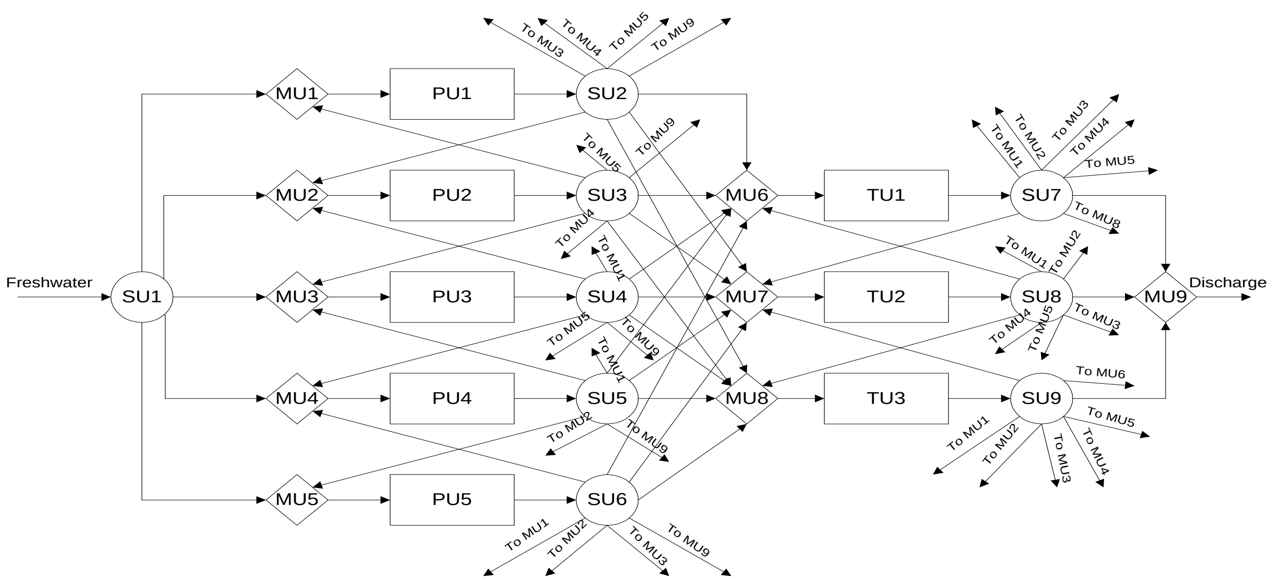

Fig. 17 Superstructure for example 4

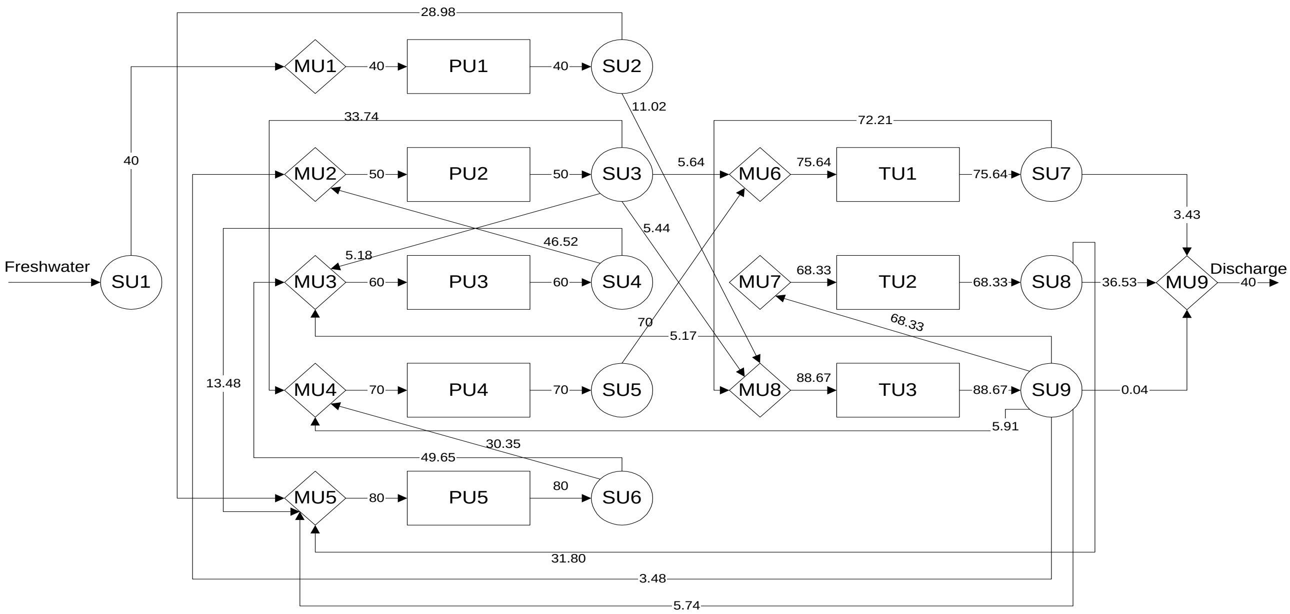

Fig. 18 Optimal solution of example 4

Computational results

Table 9a Model sizes for Examples 1 – 4

Example	Original NLP model		
	# Variables	# Constraints	# Non-convex terms
1	74	68	38
2	145	124	83
3	144	126	80
4	320	332	207

Table 9b Comparison of solution algorithms for Examples 1 – 4

Example	Local optimum (using CONOPT)	Proposed Algorithm					BARON		
		Global optimum	No. of Nodes	BCP (LP) time (sec)	Lower bounding problem (MILP) time (sec)	Total time (sec)	Global optimum	No. of Nodes	Total time (sec)
1	118.41 ton/hr	117.05 ton/hr	8	0.84	36.76	37.72	117.05 ton/hr	71	4.57
2	$ 381751.35	$ 381751.35	3	5.94	7.22	13.21	$ 381751.35	6539	597.73
3	$ 948749.07	$ 874057.37	1	1.72	0.05	1.8	-	-	> 40000
4	$ 1121848.76	$ 1033810.95	5	40.94	190.23	231.37	-	-	> 40000

Table 9a shows the sizes of the models involved in the various examples, including the number of non-convex terms. From Table 9b, it can be seen that the proposed algorithm is quite efficient, requiring about 231 CPUsecs even in the largest example. Also, it can be observed that while BARON works well for small problems, it fails to verify global optimality of the solution for large problems, even though BARON finds upper bounds which are equal to the global optima. The proposed global optimization technique is found to take a reasonable amount of computational time for both finding the upper bound and proving it to be the global optimum, even for medium and large scale systems. For instance, BARON finds the optimal solution for example 1, a network with 2 process units and 2 treatment units in about 4 CPUsecs, while the proposed algorithm takes around 37 CPUsecs. However, for the larger problem in example 4 with 5 process units and 3 treatment units, the proposed algorithm globally optimized the network in about 231 CPUsecs while BARON could not guarantee global optimality in more than 11 hrs. It is worthwhile mentioning here that if the NLP is formulated incorporating the bound strengthening cuts (eq (15)) which are redundant in the original NLP (Section 5), then

BARON performs much better than in the absence of these cuts. For instance, it finds the global optimum for the network problem with 4 process units and 2 treatment units (example 3) in just 2.13 CPUsecs when these cuts are included in the non-linear model. This illustrates the efficacy of the proposed cuts in tightening the lower bounds on the global optimum. Finally, it is also interesting to note that for large complex structures, globally optimizing the networks leads to a solution, which is significantly better than the optimum found by locally optimizing the structure. This rules in favor of globally optimizing such networks, even though deterministic global optimization techniques can be computationally expensive.

8. Selection of Treatment Technologies

In this section, we extend the network synthesis problem by allowing a choice for the treatment technology for removing a particular pollutant from the wastewater stream. Different technologies differ in their costs (Investment and Operating) and the extent of removal of the contaminants. Allowing a choice for the treatment technologies, the problem takes the form of a GDP, which is non-convex. This GDP is then reformulated as a non-convex MINLP using the convex hull representation method. The boolean variables in the GDP and the binary variables in the MINLP are associated with the discrete decisions to select one treatment technology over another. The optimization process selects the particular treatment equipment and adjusts the flows in the system such that the aggregated cost of freshwater consumption and wastewater treatment is minimized. An illustrative network superstructure with four process units and two treatment units (each unit with two possible technologies) is shown in Fig. 19.

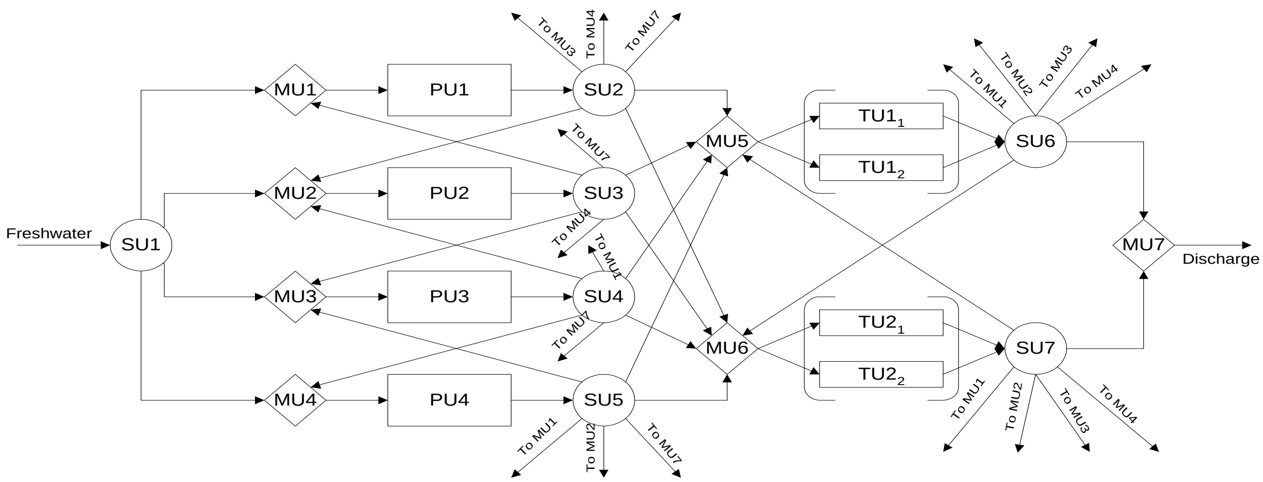

Fig. 19 Superstructure for selection of technologies for treatment units

Non-Convex GDP model

A Generalized Disjunctive Programming problem is one where a logic-based model is used to represent discrete and continuous decisions. In this integrated network synthesis problem, the logic decisions correspond to the selection of a technology out of various available choices for a treatment operation. For instance, if there are *R* choices for a technology to be used in a treatment unit *t* (with inlet stream *k* and outlet stream *i*), it can be modeled with the following set of disjunctions:

$$\bigvee_{r=1\ldots R}\begin{bmatrix} Y_{rt} \\ C^{i} = \beta^{rt} C^{k} \\ INV^{t} = \gamma^{rt}\left(F^{i}\right)^{\alpha} \\ OP^{t} = \Theta^{rt} F^{i} \\ C^{L} \le C \le C^{U} \end{bmatrix} \qquad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}$$

$$Y_{rt} \in \{true, false\}$$
$$F^{L} \le F \le F^{U}$$

where β^{rt}, γ^{rt} and Θ^{rt} are the removal ratio, investment cost coefficient and the operating cost coefficient for the r^{th} technology choice for a treatment operation denoted by *t*. If the r^{th} technology is selected, Y_{rt}, which is a Boolean variable, holds true, and the investment cost variable INV^t and the operating cost variable OP^t take on non-zero positive values. If Y_{rt} is false, all the constraints in the rth disjunct are ignored. In modeling the entire system, the equations for the mixers, splitters and process units remain the same, but the objective function and equations for treatment units have to be changed in order to account for different costs and removal ratios of the technologies. The equations in the non-convex GDP model are as follows:

Objective function: $\min \Phi = HC_{FW} FW + AR \sum_{t \in TU} INV^t + H \sum_{t \in TU} OP^t$

Mixers: $F^k = \sum_{i \in m_{in}} F^i \quad \forall m \in MU, \forall k \in m_{out}$

$$F^k C_j^k = \sum_{i \in m_{in}} F^i C_j^i \quad \forall j, \forall m \in MU, \forall k \in m_{out}$$

Splitters: $F^k = \sum_{i \in s_{out}} F^i \quad \forall s \in SU, \forall k \in s_{in}$

$$C_j^i = C_j^k \quad \forall j, \ \forall s \in SU, \forall i \in s_{out}, \forall k \in s_{in}$$

Process units: $F^k = F^i = P^p \quad \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out}$

$$P^p C_j^i + L_j^p \times 10^3 = P^p C_j^k \quad \forall j, \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out}$$

Treatment units: $F^k = F^i \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}$

$$\bigvee_{r=1\ldots R} \begin{bmatrix} Y_{rt} \\ C_j^i = \beta_j^{rt} C_j^k \quad \forall j \\ INV^t = \gamma^{rt} \left(F^i\right)^{\alpha} \\ OP^t = \Theta^{rt} F^i \\ C^L \le C \le C^U \end{bmatrix} \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}$$

$$Y_{rt} \in \{true, false\} \qquad \text{(P)}$$

$$F^L \le F \le F^U$$

Here, the boolean variables Y_{rt} stand for selection of rth treatment technology for a treatment unit denoted by *t*. Only one of the Y_{rt}'s must hold true. Using the convex hull reformulation technique (Raman and Grossmann, 1994), the given non-convex GDP is transformed into a non-convex MINLP which is then solved to global optimality.

Convex Relaxation of non-convex GDP model

Valid piecewise linear estimators are used for the relaxation of the bilinear and concave terms in the GDP problem leading to the formulation of a convex relaxed problem:

$$\min \Phi_{\mathrm{relax}} = HC_{FW} FW + AR \sum_{t \in TU} INV^t + H \sum_{t \in TU} OP^t$$

$$\begin{aligned}
s.t. \quad & F^k = \sum_{i \in m_{in}} F^i \quad \forall m \in MU, \forall k \in m_{out} \\
& f_j^k = \sum_{i \in m_{in}} f_j^i \quad \forall j, \forall m \in MU, \forall k \in m_{out} \\
& F^k = \sum_{i \in s_{out}} F^i \quad \forall s \in SU, \forall k \in s_{in} \\
& C_j^i = C_j^k \quad \forall j, \forall s \in SU, \forall i \in s_{out}, \forall k \in s_{in} \\
& F^k = F^i = P^p \quad \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out} \\
& P^p C_j^i + L_j^p \times 10^3 = P^p C_j^k \quad \forall j, \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out}
\end{aligned} \qquad \text{(R)}$$

$$
\underset{n=1\ldots N}{\vee}\left[\begin{array}{l}
W_n \\
\left\{\begin{array}{l}
f^u = \max\left\{FC^L + F_nC - F_nC^L\ ,\ FC^U + F_{n+1}C - F_{n+1}C^U\right\} \\
f^o = \min\left\{FC^L + F_{n+1}C - F_{n+1}C^L\ ,\ FC^U + F_nC - F_nC^U\right\} \\
F_n \le F \le F_{n+1}\ ,\ C^L \le C \le C^U
\end{array}\right\} \\
\underset{r=1\ldots R}{\vee}\left[\begin{array}{l}
Y_{rt} \\
F^k = F^i \\
C_j^i = \beta_j^{rt} C_j^k \qquad \forall j \\
OP^t = \Theta^{rt} F^i \\
INV^t \ge \gamma^{rt}\left\{\left(F_n^i\right)^{\alpha} + \left(\dfrac{\left(F_{n+1}^i\right)^{\alpha} - \left(F_n^i\right)^{\alpha}}{F_{n+1}^i - F_n^i}\right)\left(F^i - F_n^i\right)\right\} \\
\sum_{p \in PU} L_j^p \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \left(1 - \beta_j^{rt}\right) f_j^k + f_j^{out} \quad \forall j \\
C^L \le C \le C^U
\end{array}\right] \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in} \\
Y_{rt} \in \{true, false\} \\
W_n^a \Leftrightarrow W_n^b \quad \forall n \quad , \forall a,b \quad s.t. \quad F^a = F^b and\, F^{aL} = F^{bL} and\, F^{aU} = F^{bU}
\end{array}\right]
$$

$$
W_n \in \{true, false\}
$$
$$
F^L \le F \le F^U
$$

In model (R), all the functions are linear. It is also quite interesting to note that what we have here is a set of disjuncts within another set, i.e. a set of 'embedded disjunctions' (see Vecchietti and Grossmann, 2000). The outer disjuncts are associated with the construction of piecewise estimators while the inner ones pertain to the selection of treatment technologies. Making use of the convex hull reformulation of each disjunction we obtain the following MILP model:

$$
\min \Phi_{relax} = HC_{FW} FW + AR \sum_{t \in TU} INV^t + H \sum_{t \in TU} OP^t
$$

$$s.t. \quad F^k = \sum_{i \in m_{in}} F^i \quad \forall m \in MU, \forall k \in m_{out}$$

$$f_j^k = \sum_{i \in m_{in}} f_j^i \quad \forall j, \forall m \in MU, \forall k \in m_{out}$$

$$F^k = \sum_{i \in s_{out}} F^i \quad \forall s \in SU, \forall k \in s_{in}$$

$$C_j^i = C_j^k \quad \forall j, \ \forall s \in SU, \forall i \in s_{out}, \forall k \in s_{in}$$

$$F^k = F^i = P^p \quad \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out}$$

$$P^p C_j^i + L_j^p \times 10^3 = P^p C_j^k \quad \forall j, \forall p \in PU, \forall i \in p_{in}, \forall k \in p_{out}$$

$$F^k = F^i \quad \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}$$

$$\left(\begin{array}{l} F^i = \pi_1^i + \pi_2^i + \ldots + \pi_N^i \ ; \quad C^i = \chi_1^i + \chi_2^i + \ldots + \chi_N^i \\ F^i C^i \geq \sum_{n=1}^{N} \max\{\pi_n^i C^{iL} + F_n^i \chi_n^i - F_n^i C^{iL} \lambda_n^i \ , \pi_n^i C^{iU} + F_{n+1}^i \chi_n^i - F_{n+1}^i C^{iU} \lambda_n^i \} \\ F^i C^i \leq \sum_{n=1}^{N} \min\{\pi_n^i C^{iL} + F_{n+1}^i \chi_n^i - F_{n+1}^i C^{iL} \lambda_n^i \ , \pi_n^i C^{iU} + F_n^i \chi_n^i - F_n^i C^{iU} \lambda_n^i \} \\ F_n^i \lambda_n^i \leq \pi_n^i \leq F_{n+1}^i \lambda_n^i \ ; \ C^{iL} \lambda_n^i \leq \chi_n^i \leq C^{iU} \lambda_n^i \qquad\qquad n = 1, \ldots, N \\ \sum_{n=1}^{N} \lambda_n^i = 1 \, ; \, \lambda_n^i \in \{0,1\} \end{array} \right) \quad \forall m \in MU, \forall i \in m_{in}, \forall i \in m_{out}, \forall i \notin t_{in}, \forall i \notin t_{out}$$

$$\left(\begin{array}{l} F^i = \sum_{n=1}^{N} \sum_{r=1}^{R} \eta_{rn}^i \ ; \quad C^i = \sum_{n=1}^{N} \sum_{r=1}^{R} \psi_{rn}^i \\ F^i C^i \geq \sum_{n=1}^{N} \sum_{r=1}^{R} \max\{\eta_{rn}^i C^{riL} + F_{rn}^i \psi_{rn}^i - F_{rn}^i C^{riL} w_{rn}^t \ , \eta_{rn}^i C^{riU} + F_{r(n+1)}^i \psi_{rn}^i - F_{r(n+1)}^i C^{riU} w_{rn}^t \} \\ F^i C^i \leq \sum_{n=1}^{N} \sum_{r=1}^{R} \min\{\eta_{rn}^i C^{riL} + F_{r(n+1)}^i \psi_{rn}^i - F_{r(n+1)}^i C^{riL} w_{rn}^t \ , \eta_{rn}^i C^{riU} + F_{rn}^i \psi_{rn}^i - F_{rn}^i C^{riU} w_{rn}^t \} \\ INV^t \geq \sum_{n=1}^{N} \sum_{r=1}^{R} \gamma^{rt} \left(\left(F_{rn}^i\right)^{\alpha} w_{rn}^t + \left(\frac{\left(F_{r(n+1)}^i\right)^{\alpha} - \left(F_{rn}^i\right)^{\alpha}}{F_{r(n+1)}^i - F_{rn}^i} \right) \left(\eta_{rn}^i - F_{rn}^i w_{rn}^t \right) \right) \qquad r = 1, \ldots, R \\ OP^t = \sum_{r=1}^{R} \Theta^{rt} F^{ri} \\ F_{rn}^i w_{rn}^t \leq \eta_{rn}^i \leq F_{r(n+1)}^i w_{rn}^t \ ; \ C^{riL} w_{rn}^t \leq \psi_{rn}^i \leq C^{riU} w_{rn}^t \qquad\qquad r = 1, \ldots, R \quad , n = 1, \ldots, N \\ \sum_{n=1}^{N} \sum_{r=1}^{R} w_{rn}^t = 1 \, ; \, w_{rn}^t \in \{0,1\} \end{array} \right) \quad \forall t \in TU, \forall i \in t_{in}, \forall i \in t_{out}$$

$$F^i = \sum_{r=1}^{R} F^{ri} \quad \forall t \in TU, \forall i \in t_{out}$$

$$F^k = \sum_{r=1}^{R} F^{rk} \quad \forall t \in TU, \forall k \in t_{in}$$

$$F^{riL} y_{rt} \leq F^{ri} \leq F^{riU} y_{rt} \quad \forall t \in TU, \forall i \in t_{out}, r = 1 \ldots R$$

$$F^{rkL} y_{rt} \leq F^{rk} \leq F^{rkU} y_{rt} \quad \forall t \in TU, \forall k \in t_{in}, r = 1 \ldots R$$

$$
\begin{aligned}
& f_j^k = \sum_{r=1}^{R} f_j^{rk} \qquad \forall j, \forall t \in TU, \forall k \in t_{in} \\
& \sum_{p \in PU} L_j^p \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \sum_{r=1}^{R} \left(1 - \beta_j^{rt}\right) f_j^{rk} + f_j^{out} \quad \forall j \\
& f_j^{rkL} y_{rt} \le f_j^{rk} \le f_j^{rkU} y_{rt} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}, r = 1 \dots R \\
& C_j^i = \sum_{r=1}^{R} C_j^{ri} \qquad \forall j, \forall t \in TU, \forall i \in t_{out} \\
& C_j^k = \sum_{r=1}^{R} C_j^{rk} \qquad \forall j, \forall t \in TU, \forall k \in t_{in} \\
& C_j^{ri} = \beta_j^{rt} C_j^{rk} \qquad \forall j, \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}, r = 1 \dots R \\
& C_j^{riL} y_{rt} \le C_j^{ri} \le C_j^{riU} y_{rt} \qquad \forall j, \forall t \in TU, \forall i \in t_{out}, r = 1 \dots R \\
& C_j^{rkL} y_{rt} \le C_j^{rk} \le C_j^{rkU} y_{rt} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}, r = 1 \dots R \\
& \sum_{r=1}^{R} y_{rt} = 1 \,;\, y_{rt} \in \{0,1\} \qquad \forall t \in TU \\
& \sum_{n=1}^{N} w_{rn}^{t} = y_{rt} \qquad \forall t \in TU, r = 1 \dots R \\
& \lambda_n^a = \lambda_n^b \quad \forall n, \quad \forall a,b \quad s.t. \quad F^a = F^b \, and \; F^{aL} = F^{bL} and \; F^{aU} = F^{bU} \\
& F^L \le F \le F^U, \quad C^L \le C \le C^U
\end{aligned}
\qquad \text{(R-CH)}
$$

In this formulation, F_{rn} (n = 1, …, N) are the intermediate points used to divide the space between F^{rL} and F^{rU}. The optimal solution of this MILP provides a valid lower bound to the optimal solution of problem (P) since the relaxed MILP problem has been created by convexifying the feasible region of the original GDP problem (P). This approach of convexifying a MINLP using linear estimators for the non-convex functions, and enforcing the integrality of the discrete variables to obtain a lower bounding MILP problem, has also been suggested by other authors, for instance by Smith and Pantelides (1997).

Bounds Tightening

We use a bound contraction technique to tighten the bounds of the complicating variables, which greatly affect the quality of the convex relaxation (R-CH). The model that is solved here is a modified version of the model (P) with the non-convex terms being approximated with linear estimators, the objective function changed and an additional constraint being introduced. Moreover, the integrality constraints on the discrete variables are relaxed in the bound contraction model (B-CH), yielding the LP subproblem,

$$\min / \max \ F^i$$

s.t.

$$HC_{FW}FW + AR\sum_{\substack{t\in TU\\ i\in t_{out}}}\sum_{r=1}^{R}\gamma^{rt}\left(\left(F^{riL}\right)^{\alpha}y_{rt} + \left(\frac{\left(F^{riU}\right)^{\alpha}-\left(F^{riL}\right)^{\alpha}}{F^{riU}-F^{riL}}\right)\left(F^{ri}-F^{iL}y_{rt}\right)\right) + H\sum_{\substack{t\in TU\\ i\in t_{out}}}\sum_{r=1}^{R}\Theta^{rt}F^{ri} \le OUB$$

$$F^k = \sum_{i\in m_{in}} F^i \quad \forall m\in MU, \forall k\in m_{out}$$

$$f_j^k = \sum_{i\in m_{in}} f_j^i \quad \forall j, \forall m\in MU, \forall k\in m_{out}$$

$$F^k = \sum_{i\in s_{out}} F^i \quad \forall s\in SU, \forall k\in s_{in}$$

$$C_j^i = C_j^k \quad \forall j,\ \forall s\in SU, \forall i\in s_{out}, \forall k\in s_{in}$$

$$F^k = F^i = P^p \quad \forall p\in PU, \forall i\in p_{in}, \forall k\in p_{out}$$

$$P^p C_j^i + L_j^p\times 10^3 = P^p C_j^k \quad \forall j, \forall p\in PU, \forall i\in p_{in}, \forall k\in p_{out}$$

$$F^k = F^i \quad \forall t\in TU, \forall i\in t_{out}, \forall k\in t_{in}$$

$$F^i = \sum_{r=1}^{R} F^{ri} \qquad \forall t\in TU, \forall i\in t_{out}$$

$$F^k = \sum_{r=1}^{R} F^{rk} \qquad \forall t\in TU, \forall k\in t_{in}$$

$$F^{riL}y_{rt} \le F^{ri} \le F^{riU}y_{rt} \qquad \forall t\in TU, \forall i\in t_{out}, r=1\ldots R$$

$$F^{rkL}y_{rt} \le F^{rk} \le F^{rkU}y_{rt} \qquad \forall t\in TU, \forall k\in t_{in}, r=1\ldots R$$

$$C_j^i = \sum_{r=1}^{R} C_j^{ri} \qquad \forall j, \forall t \in TU, \forall i \in t_{out}$$

$$C_j^k = \sum_{r=1}^{R} C_j^{rk} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}$$

$$C_j^{ri} = \beta_j^{rt} C_j^{rk} \quad \forall j, \forall t \in TU, \forall i \in t_{out}, \forall k \in t_{in}, r = 1 \ldots R$$

$$C_j^{riL} y_{rt} \le C_j^{ri} \le C_j^{riU} y_{rt} \qquad \forall j, \forall t \in TU, \forall i \in t_{out}, r = 1 \ldots R$$

$$C_j^{rkL} y_{rt} \le C_j^{rk} \le C_j^{rkU} y_{rt} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}, r = 1 \ldots R$$

$$f_j^k = \sum_{r=1}^{R} f_j^{rk} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}$$

$$\sum_{p \in PU} L_j^p \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \sum_{r=1}^{R} \left(1 - \beta_j^{rt}\right) f_j^{rk} + f_j^{out} \quad \forall j$$

$$f_j^{rkL} y_{rt} \le f_j^{rk} \le f_j^{rkU} y_{rt} \qquad \forall j, \forall t \in TU, \forall k \in t_{in}, r = 1 \ldots R$$

$$\sum_{r=1}^{R} y_{rt} = 1 \,;\, 0 \le y_{rt} \le 1 \qquad \forall t \in TU$$

$$\begin{pmatrix} f_j^i \ge F^{iL} C_j^i + C_j^{iL} F^i - F^{iL} C_j^{iL} \\ f_j^i \ge F^{iU} C_j^i + C_j^{iU} F^i - F^{iU} C_j^{iU} \\ f_j^i \le F^{iL} C_j^i + C_j^{iU} F^i - F^{iL} C_j^{iU} \\ f_j^i \le F^{iU} C_j^i + C_j^{iL} F^i - F^{iU} C_j^{iL} \end{pmatrix} \qquad \forall j, \forall m \in MU, \forall i \in m_{in}, \forall i \in m_{out}, \forall i \notin t_{in}, \forall i \notin t_{out}$$

$$\begin{pmatrix} f_j^i \ge \sum_{r=1}^{R} \left(F^{riL} C_j^{ri} + C_j^{riL} F^{ri} - F^{riL} C_j^{riL}\right) \\ f_j^i \ge \sum_{r=1}^{R} \left(F^{riU} C_j^{ri} + C_j^{riU} F^{ri} - F^{riU} C_j^{riU}\right) \\ f_j^i \le \sum_{r=1}^{R} \left(F^{riL} C_j^{ri} + C_j^{riU} F^{ri} - F^{riL} C_j^{riU}\right) \\ f_j^i \le \sum_{r=1}^{R} \left(F^{riU} C_j^{ri} + C_j^{riL} F^{ri} - F^{riU} C_j^{riL}\right) \end{pmatrix} \qquad \forall j, \forall t \in TU, \forall i \in t_{in}, \forall i \in t_{out} \tag{B-CH}$$

$$F^L \le F \le F^U, \quad C^L \le C \le C^U$$

9. Global optimization of non-convex GDP models

The basic steps of the proposed global optimization algorithm remain the same as those given in Section 6, with the only difference lying in the model equations being optimized. Here, models (B-CH), (R-CH) presented in the previous section, which correspond to the LP formulation of the bound contraction problem and the MILP formulation of the lower bounding problem respectively, are solved in steps 1 and 2 respectively of the proposed method. The only two other changes in the given algorithm are as follows,

a. In *Step 0*, the MINLP reformulation of the model (P) is solved instead of an NLP, to obtain an overall upper bound on the objective function.
b. For calculating the upper bound (*Step 4*), we fix the values of the binary variables in the MINLP reformulation of model (P), to the optimal values obtained from the solution of the lower bounding problem. Hence the non-convex MINLP is converted into a non-convex NLP that is locally optimized for determining the upper bound.

The branching is carried out on the continuous variables as in the case of global optimization of continuous NLPs. This methodology for solving the design problem with the option of selecting one out of various treatment technologies is then applied to optimize a network similar in structure to that in example 3.

<u>Example 5</u> We consider an integrated network with 4 process units and 2 treatment units (superstructure in Fig. 19). Like example 3, this is a two contaminant system with the environmental discharge limits on the contaminant concentrations being 10 ppm. The data for freshwater cost, annualized factor for investment and hours of plant operation per annum were also taken from example 3. There is a choice of two different technologies for each treatment unit in the system: $TU1_1$ and $TU1_2$ for treatment unit *TU1* and $TU2_1$ and $TU2_2$ for the unit *TU2*. One treatment technology for each treatment unit is chosen by the optimization method, which leads to the minimum annual cost. The process and treatment unit data for the optimization are taken from Table 5 and Table 10, respectively.

Table 10. Treatment Unit data for Example 5

Unit #	Treatment technology	Removal ratio (%) A	B	IC (Investment Cost Coefficient)	OC (Operating Cost Coefficient)	α
TU1	$TU1_1$	95	0	16800	1	0.7
	$TU1_2$	90	0	4800	0.5	0.7
TU2	$TU2_1$	0	90	12600	0.0067	0.7
	$TU2_2$	0	95	36000	0.067	0.7

The problem size is shown in Table 11a, while the computational results are tabulated in Table 11b.

Table 11a Problem size for Example 5

Example	Original MINLP model			
	# Continuous Variables	# Binary Variables	# Constraints	#Non-convex terms
4	178	4	190	82

Table 11b Computational results for Example 5

Example	Local optimum (using DICOPT)	Proposed Algorithm					BARON		
		Global optimum	No. of Nodes	BCP (LP) time (sec)	Lower bounding problem (MILP) time (sec)	Total time (sec)	Global optimum	No. of Nodes	Total time (sec)
4	$ 665,827.72	$ 619,205.4	1	1.72	0.53	2.27	$ 619,205.4	37621	17541

Fig. 20 shows the optimal network structure for this example, indicating the treatment technology that is selected for each treatment process. It can be observed from Table 11b that the global solution of $ 619,205.4 is considerably lower than the suboptimal solution of $ 665,827.72 found by DICOPT++. The use of BARON to solve the non-convex MINLP does yield the global optimum, but takes a much longer time (17,541 CPUsecs) as compared to the proposed technique (2.27 CPUsecs). On using the proposed algorithm, the lower and upper bounds converge within the specified tolerance at the root node itself.

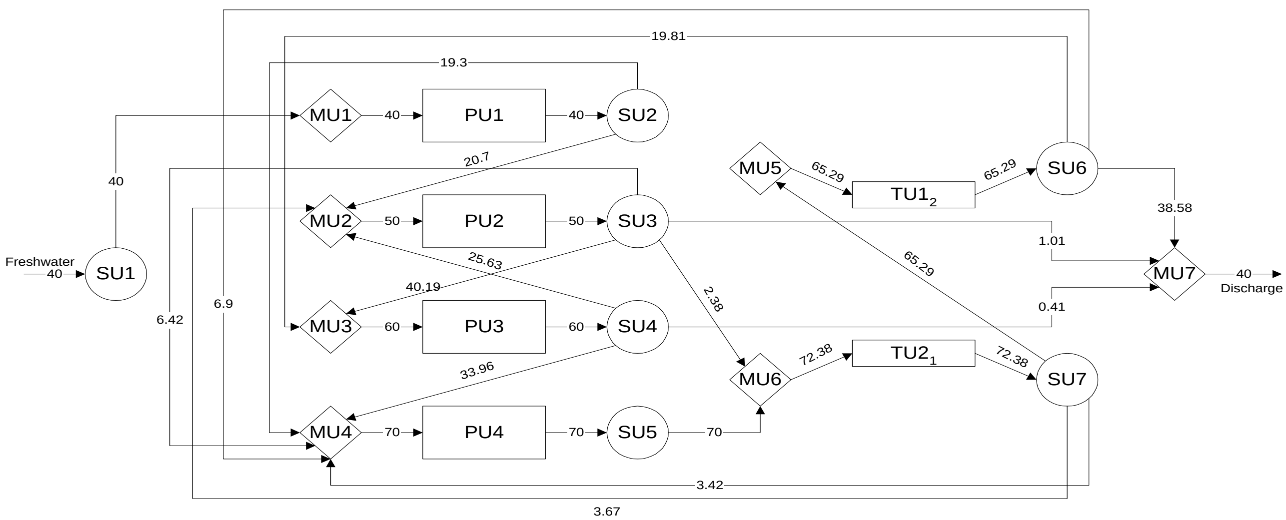

Fig. 20 Optimal solution of Example 5

10. Conclusions

In this paper we have presented a superstructure for synthesizing a minimum cost integrated water system consisting of water using and water treating units, and illustrated with the help of an example, the advantage of constructing and optimizing integrated networks over separately optimizing different sets of water using and treatment operations. Initially, the integrated system is formulated as a continuous NLP problem since all the process and treatment units in the network are fixed. We have proposed a new Spatial Branch and Contract algorithm for the global optimization of such networks. Tight lower bounds on the global optimum are obtained from a convex relaxation of the original problem by approximating the non-convex terms in the NLP model with piecewise linear estimators. We have also modeled the network as a GDP problem by allowing a choice for different treatment technologies for the operation of a single treatment unit. The convex hull relaxation of this GDP results in an MINLP problem, which is solved to global optimality with a modified version of the proposed algorithm. Numerical results of the application of the global optimization technique on various examples have been presented. The proposed method was found to perform better computationally for large-scale problems as compared to the general purpose solver BARON. The study of such integrated networks can be further extended by taking into account the cost of piping in these structures and also by modeling the water treating units with non-linear equations.

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