Global Optimization of Multiscenario Mixed Integer Nonlinear Programming Models arising in the Synthesis of Integrated Water Networks under Uncertainty

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ABSTRACT

The problem of optimal synthesis of an integrated water system is addressed in this work, where water using processes and water treatment operations are combined into a single network such that the total cost of building the network, and operating it optimally is globally minimized. The network has to be designed to be feasible and optimal over a given set of scenarios in which different operational conditions hold. The uncertain operational parameters in the system are the amount of contaminants generated in the process units and the extent of removal of the contaminants inside the treatment units. We optimize a superstructure that incorporates all feasible design alternatives for wastewater treatment, reuse and recycle, with a multiscenario nonconvex Mixed Integer Non-Linear Programming (MINLP) model, which is a deterministic equivalent of a two-stage stochastic programming model with recourse, and where the uncertain parameters take on a finite number of realizations. These models can grow in size with the number of scenarios and often require exponential computational effort to be solved to rigorous global optimality. To effectively solve this problem, we propose a spatial branch and cut algorithm that uses Lagrangean decomposition for global optimization of the large multiscenario model. Two examples are presented to illustrate the global optimization of integrated water networks under uncertainty using the proposed algorithm.

Keywords: Global optimization; Integrated water networks; Nonconvex MINLP; Uncertainty; Lagrangean cuts

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1. INTRODUCTION

Process synthesis under uncertainty is in general a very challenging problem. There are usually a number of parameters which may change during the operation of a process network and for which the data is not known exactly. Therefore, a major objective when synthesizing a network operating under uncertainty is that the design should be optimal and feasible over a range of values of these uncertain parameters. Two major approaches for achieving this objective are the one based on flexibility and the one based on stochastic programming. In the former, the stress is on ensuring feasibility of design by adjusting the control variables in the system when the uncertain parameters change (Grossmann et al., 1983). In a stochastic programming approach (Birge and Louveaux, 1997), the emphasis is on achieving optimality accounting for the fact that the recourse variables can be adjusted for each parameter realization (see Acevedo and Pistikopolous, 1998; Clay and Grossmann, 1997; and Liu and Sahinidis, 1996). Both approaches can be considered to be equivalent if the goals of optimality and feasibility are simultaneously achieved. In a two stage stochastic programming approach, the 1^{st} stage or "here and now" decisions (taken prior to the appearance of uncertainty) have to be taken such that the expected costs of the 2^{nd} stage (costs of operating the network after the uncertainty has presented itself) are minimized. There exist numerous methods for the solution of several classes of stochastic programs (Takriti et al., 1996; Ahmed et al., 2004; Norkin et al., 1998). A recent review of the major techniques for optimization under uncertainty is given in Sahinidis (2004).

For process synthesis problems under uncertainty, usually it can be assumed that the uncertain parameters take on a finite set of known values, and hence one can postulate a finite number of scenarios to characterize the uncertainty by allowing the uncertain parameters to take on different values in different scenarios. In this way, a general two stage stochastic programming problem can be formulated as an equivalent deterministic multiscenario mathematical program. The deterministic multiscenario model for a process synthesis problem, where the uncertain parameters take on a finite set of values is as follows:

$$
\begin{aligned}
&\min_{d,x_n} \; z = f^0(d) + \sum_n p_n f_n(x_n,\theta_n) \\
&s.t. \quad \left.\begin{aligned} h_n(d,x_n,\theta_n) = 0 \\ g_n(d,x_n,\theta_n) \le 0 \end{aligned}\right\} n \in N \\
&\qquad d \in D, x_n \in X, \theta_n \in \Theta
\end{aligned}
$$

Here d corresponds to the first stage design variables, x_n and θ_n are the vector of the second stage state variables and the vector of uncertain parameters in scenario $n \in$ N, respectively, while p_n is the probability assigned to the occurrence of the nth scenario. Some of the state variables are control variables, which can be manipulated during network operation such that the network operates optimally even when the uncertain parameters change. It is important to note that the design variable vector, d, has to be chosen in the first stage and cannot be changed in the second stage when the network is being operated. The number of scenarios in the model is given by $|N|$. The equality constraints h_n normally correspond to the mass and energy balances in each scenario while the inequalities g_n usually correspond to the design specifications and logical constraints. Further, in the objective function, $f^0(d)$ is the capital cost of the design while $\sum_n p_n f_n(x_n, \theta_n)$ is the total expected operating cost of the system over all the scenarios which is highly dependent on the choice of the first stage design variables.

In this paper we address the problem of designing integrated water networks operating under uncertain operational conditions. This is an extension of an earlier work by Karuppiah and Grossmann (2006a), which deals with the synthesis of globally optimized integrated water networks, operating under steady state conditions without any uncertainty. In this work, we consider a number of uncertain parameters in the system that change during the duration of operation of the network. A two stage stochastic programming framework is used to formulate the design problem. This problem is reformulated as a deterministic multiscenario Mixed Integer Non-Linear Programming (MINLP) problem since the uncertain parameters can take on a finite number of realizations and are assumed to do so in a finite set of scenarios. In this approach, the duration of operation of the integrated water network is divided into a finite set of scenarios where the uncertain parameters can take on different values in each scenario. A similar problem has been considered by Al-Redhwan et al. (2005) where the authors use a scenario approach to represent the uncertainty in the system. They minimize the wastewater flows from different processes in a plant where the operational conditions are subject to uncertainty, and obtain local solutions. The effects the piping and investment cost for the design of the network is not taken into account.

Usually the multiscenario models grow in size with the number of scenarios ($|N|$) and are computationally expensive to solve. In this work, a spatial branch and cut algorithm is proposed to solve the multiscenario MINLP model corresponding to the design problem to global optimality. In this approach, cuts based on Lagrangean decomposition of the problem are generated and added to the original problem to strengthen the convex relaxation of the original nonconvex model so as to accelerate the convergence of the spatial branch and bound algorithm. Two examples are presented to illustrate that the algorithm is effective in solving the large multiscenario models in significantly less time than BARON (Sahinidis, 1996), which is a global optimization solver for MINLPs.

2. PROBLEM STATEMENT

In this paper, we consider the optimal synthesis of an integrated water network (see Karuppiah and Grossmann, 2006a), consisting of water using process units (e.g. reactors, washing units), water treatment units (e.g. membranes, centrifuges) and mixers and splitters, operating under uncertain operational conditions. In order to systematically consider all the design alternatives, a superstructure of an integrated water system is constructed with various interconnections between all the units and globally optimized to obtain a minimum cost network. The superstructure of an illustrative water network with two process units and two treatment units is shown in Fig. 1.

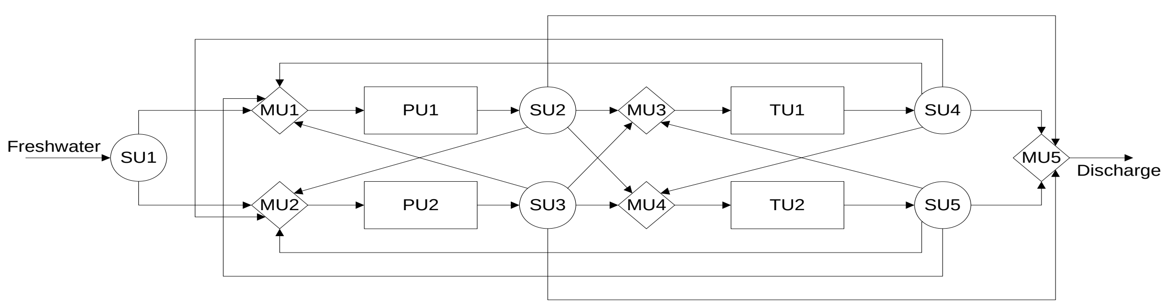

Fig. 1 Superstructure of integrated network with 2 Process units and 2 Treatment units

A detailed description for deriving superstructures of these integrated water networks is given in Karuppiah and Grossmann (2006a). The basic idea is that there are a set of water using process units with fixed demand of water, which is met by a freshwater source or wastewater coming from other processes. There is also a limit on the contaminant concentrations in the inlet streams to the process units. The wastewater generated in all the water using processes is treated in a set of water treatment units from where it is either discharged into the environment or recycled back for use in the water using operations. The contaminant levels in the discharge must fall below specified limits.

The integrated process water networks are subjected to significant uncertainties in the contaminant loads generated inside the process units and the contaminant removals in the treatment units. These are uncertain parameters which take on different values at different points of time during network operation. Because the integrated network is highly interconnected, changes in the uncertain parameters can adversely affect all parts of the network and it may not be possible to operate the network without violating the discharge restrictions or the contaminant levels in the inlets to the process units. To avoid this situation, the effect of uncertainty in the contaminant loads and the contaminant removals has to be taken into account at the time of designing the network. Hence we formulate the design problem as a two stage stochastic programming problem. In the first stage, the network is selected and in the second stage the network is operated. The objective is to construct a network such that the total costs of designing the network and the expected cost of operating the network optimally over the entire duration of operation is minimized. The first stage capital costs include the investment cost for piping which depends on the maximum flowrate allowable in a pipe, and the capital cost of each treatment unit, which is dependent on the maximum flow of wastewater to be handled by that treatment unit. The operating costs of the network appear in the second stage, which include the cost of obtaining freshwater for use in the process units, the cost of pumping a certain flow of water through the pipes (this flow should be less than the maximum flow allowable in the pipes) and the operating costs of treating wastewater in the treatment units.

Decisions pertaining to the first stage which are taken prior to the appearance of uncertainty in the system are, (i) whether a piping connection should exist between two pieces of equipment, (ii) the maximum water flowrate allowed in each pipeline and, (iii) the maximum volume of wastewater to be treated in each treatment unit. These decisions correspond to the design variables in the problem and once chosen, these design variables remain fixed throughout the duration of operation of the network and cannot be altered during operation. The second stage decisions are the flows of water to be pumped through each pipe in the network and the freshwater to be consumed at various times during operation. These can be changed during network operation depending on the values taken by the uncertain parameters. The problem is to mathematically model the network and optimize the model so as to determine the optimal first and second stage decisions that globally minimize the total cost of the network.

3. MODEL

In order to mathematically model the network operating under uncertainty, we first represent the uncertainty in the system through the use of scenarios. The operation of the network is divided into |N| different scenarios, where it is assumed that the uncertain parameters take on different known values. Further, probabilities are assigned to the occurrence of each scenario. The model equations have to ensure that the flow balances in each unit have to hold in every scenario and also the contaminant concentrations in the discharge stream and the in the inlet streams to the process units have to fall below specified limits in each scenario. Some of the assumptions involved in modeling the system are:

(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) There is no loss of water inside the process units or the treatment units

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

We extend the nonconvex NLP formulation for the synthesis of integrated water networks given in Karuppiah and Grossmann (2006a) to formulate the multiscenario MINLP model.

Objective function: The aim is to minimize the sum of the capital costs (incurred only once at the time of building the network) and the operating costs of the network which are incurred during each scenario $n \in$ N. The objective function is given as follows:

$$\min z^P = AR\left[\sum_i \left(C_p^i y^i + IP^i\left(\hat{F}^i\right)^{\delta}\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t\left(\hat{F}^i\right)^{\alpha} + H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n + H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i \tag{1}$$

where, H = Hours of operation of plant per annum (hr/ yr)

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

AR = Annualized factor for investment on treatment units and pipes (/yr)

C_p^i = Cost coefficient corresponding to existence of pipe i (\$)

FW_n = Freshwater intake into the system in scenario n (ton/ hr)

$IP^i\,(\hat{F}^i)^\delta$ = Investment cost of a pipe i (\$)

$IC^t\,(\hat{F}^i)^\alpha$ = Investment cost of a treatment unit t with outlet stream i (\$)

$PM^i F_n^i$ = Cost of pumping water inside a pipe i in scenario n (\$/ hr)

$OC^t F_n^i$ = Operating cost of a treatment unit t with outlet stream i (\$/ hr)

p_n = Probability of occurrence of scenario n.

The binary design variable y^i pertains to the existence of a stream/pipe i. The continuous first stage design variable $\hat{F}^i$ pertains to the maximum flow allowable in a pipe i while the vector F_n^i is the second stage state variable, which corresponds to the water flow in the pipe i, during scenario n. The second stage state variables implicitly depend on the first stage design variables, and hence the second stage operating costs are also implicitly dependent on the first stage decisions. The individual terms $AR\sum_i\left(C_p^i y^i + IP^i\left(\hat{F}^i\right)^\delta\right)$ and $AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t\left(\hat{F}^i\right)^\alpha$ constitute the first stage capital costs while $H\sum_n p_n \sum_i PM^i F_n^i \;+\; H\sum_n p_n C_{FW} FW_n \;+\; H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i$ is the second stage expected operating cost.

Mixer Units: The overall mass balances and individual contaminant balances for a mixer unit $m \in$ MU with a set of inlet streams $i \in m_{in}$, and an outlet stream $k \in m_{out}$ are given in eqs (2) and (3), respectively. Eq (2) contains bilinear terms which are a source of nonconvexity of the optimization model. The material balances have to hold for each scenario $n \in$ N. Here, C_{jn}^i is the concentration of contaminant j (in ppm) in stream i in scenario n.

$$F_n^k = \sum_{i\in m_{in}} F_n^i \qquad \forall m \in MU\,,\, k \in m_{out}\,,\forall n \in N \tag{2}$$

$$F_n^k C_{jn}^k = \sum_{i\in m_{in}} F_n^i C_{jn}^i \qquad \forall j, \forall m \in MU, k \in m_{out}, \forall n \in N \tag{3}$$

All the flows (F_n^i), and contaminant concentrations (C_{jn}^i) in the system are non-negative and lie within specified bounds.

Splitter Units: The splitter units $s \in$ SU consist of an inlet stream $k \in s_{in}$ and a set of outlet streams i specified in the index set s_{out}. The overall flow balances and the component balances for these units for each scenario are given in eqs (4) and (5) respectively.

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

$$C_{jn}^i = C_{jn}^k \quad \forall j, \forall s \in SU, \forall i \in s_{out}, k \in s_{in}, \forall n \in N \tag{5}$$

Process Units: The mass balance equations for every scenario, for a process unit $p \in$ PU with an inlet stream $i \in p_{in}$ and an outlet stream $k \in p_{out}$ are shown in eqs (6) and (7), where eqn (6) corresponds to the overall flow balance and eqn (7) to the individual component balance. The contaminant loads of each contaminant j inside the process units, given by L_j^p (in kg / hr), are a source of uncertainty in the network and take on different values in each scenario n.

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

$$P^p C_{jn}^i + L_{jn}^p \times 10^3 = P^p C_{jn}^k \quad \forall j, \forall p \in PU, i \in p_{in}, k \in p_{out}, \forall n \in N \tag{7}$$

Treatment Units: Equations (8) and (9) describe the flow balance and the contaminant concentration balance for all the scenarios for a treatment unit $t \in$ TU with an inlet stream $k \in t_{in}$ and an outlet stream $i \in t_{out}$.

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

$$C_{jn}^i = \beta_{jn}^t C_{jn}^k \quad \forall j, \forall t \in TU, i \in t_{out}, k \in t_{in}, \forall n \in N \tag{9}$$

The contaminant removal ratios in the treatment units are different in each scenario n. The parameter β_j^t = 1 – {(Removal ratio for contaminant j in unit t (in %)) / 100} and it takes on different values in each scenario n $\left(\beta_{jn}^t\right)$. All the uncertain parameters in the system are assumed to be independent of each other.

Bound strengthening cuts: We add valid constraints to the original model based on contaminant balances for the overall system in order to strengthen the convex relaxation of the multiscenario MINLP model (see Karuppiah and Grossmann, 2006a).

$$\sum_{p \in PU} L_{jn}^p \times 10^3 = \sum_{\substack{t \in TU \\ k \in t_{in}}} \left(1 - \beta_{jn}^t\right) F_n^k C_{jn}^k + F_n^{out} C_{jn}^{out} \quad \forall j, \forall n \in N \tag{10}$$

where, F_n^{out} and C_{jn}^{out} are the flow and concentration of contaminant j in the outlet stream to the environment, respectively, in scenario n.

Design Constraints: These constraints relate the design variables y^i and $\hat{F}^i$ (shown in eq (11)).

$$\hat{F}^{iL} y^i \le \hat{F}^i \le \hat{F}^{iU} y^i \qquad \forall i \qquad (11)$$

These simply imply that if a pipe exists, the maximum flow in it can take a value between the specified bounds, while if it does not exist, the maximum flow for that pipe goes to zero.

Linking constraints: The "hard" constraints that link the variables of each scenario with the design variables are given in eq (12). Physically, these constraints mean that the design variable $\hat{F}^i$, which is the maximum flow allowable in a pipe *i*, has to be greater than the flow in that pipe *i* in every scenario $n \in$ N (given by F_n^i).

$$\hat{F}^i \ge F_n^i \qquad \forall i, \forall n \in N \qquad (12)$$

The multiscenario MINLP model (P) comprises equations (1) – (12) which is to be globally optimized. On solving this model, we obtain the values of the design variables which define the network topology, and we also obtain the values of the control variables ($F_n^i \quad \forall i, \forall n \in N$), which are the flows of water to be pumped in each pipe *i*, in every scenario *n*. The values of the state variables, which are the contaminant concentration in all the streams in the network in each scenario, are also obtained as a result of the optimization.

4. SOLUTION METHOD

The multiscenario model such as problem (P) grows quickly in size with the number of scenarios and is very difficult to solve to global optimality without the help of specialized techniques. We propose a spatial branch and cut algorithm to solve the multiscenario MINLP to global optimality. Lower bounds are obtained at every node of the tree by solving a convex relaxation of model (P) with certain cuts added to it. In order to generate cuts, a decomposition scheme is proposed, where we use Lagrangean relaxation to decompose the nonconvex model (P) into single scenario sub-problems at every node of the search tree. These sub-problems are then solved to global optimality and their solutions are used to generate the bound strengthening cuts. A heuristic is used for the generation of good upper bounds at each node. The lower and upper bounds are then converged to within a specified tolerance in the branch and cut algorithm.

4.1. Generation of tight lower bounds: Lower bounds on the solution of (P) at every node of the branch and bound tree can be obtained by solving a convex relaxation of the nonconvex MINLP model (P). This relaxation is obtained by convexifying the nonconvex terms in model (P) with linear under- and over-estimators. The bilinear terms in the constraint set of model (P) are replaced by convex envelopes (McCormick, 1976), while the concave terms appearing in the objective function can be underestimated by secant functions. Some techniques for constructing convex estimators of various nonconvex functions are given in Quesada and Grossmann (1995), Ryoo and Sahinidis (1995) and Tawarmalani and Sahinidis (2002). Replacing the nonconvex terms in (P) with linear estimators yields a Mixed Integer Linear Programming (MILP) relaxation denoted by (CR).

$$\min z^{CR} = AR\left[\sum_i \left(C_p^i y^i + IP^i \tilde{F}^i\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t \overline{F}^i + H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n \ + \ H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i$$

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

$$f_{jn}^k = \sum_{i\in m_{in}} f_{jn}^i \quad \forall j, \forall m\in MU, k\in m_{out}, \forall n\in N$$

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

$$C_{jn}^i = C_{jn}^k \qquad \forall j, \forall s\in SU, \forall i\in s_{out}, k\in s_{in}, \forall n\in N$$

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

$$P^p C_{jn}^i + L_{jn}^p \times 10^3 = P^p C_{jn}^k \quad \forall j, \forall p\in PU, i\in p_{in}, k\in p_{out}, \forall n\in N$$

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

$$C_{jn}^i = \beta_{jn}^t C_{jn}^k \quad \forall j, \forall t\in TU, i\in t_{out}, k\in t_{in}, \forall n\in N$$

$$\sum_{p\in PU} L_{jn}^p \times 10^3 = \sum_{\substack{t\in TU\\ k\in t_{in}}} \left(1-\beta_{jn}^t\right) f_{jn}^k + f_{jn}^{out} \quad \forall j, \forall n\in N$$

$$\hat{F}^{iL} y^i \le \hat{F}^i \le \hat{F}^{iU} y^i \qquad \forall i$$

$$\hat{F}^i \ge F_n^i \qquad \forall i, \forall n\in N$$

$$\left.\begin{aligned} f_{jn}^i &\ge F_n^{iL} C_{jn}^i + C_{jn}^{iL} F_n^i - F_n^{iL} C_{jn}^{iL}\\ f_{jn}^i &\ge F_n^{iU} C_{jn}^i + C_{jn}^{iU} F_n^i - F_n^{iU} C_{jn}^{iU}\\ f_{jn}^i &\le F_n^{iL} C_{jn}^i + C_{jn}^{iU} F_n^i - F_n^{iL} C_{jn}^{iU}\\ f_{jn}^i &\le F_n^{iU} C_{jn}^i + C_{jn}^{iL} F_n^i - F_n^{iU} C_{jn}^{iL} \end{aligned}\right\} \quad \forall j, \forall m\in MU, \forall i\in \{m_{in}\cup m_{out}\}, \forall n\in N$$

$$\overline{F}^i \ge \left(\hat{F}^{iL}\right)^\alpha + \left(\frac{\left(\hat{F}^{iU}\right)^\alpha - \left(\hat{F}^{iL}\right)^\alpha}{\hat{F}^{iU} - \hat{F}^{iL}}\right)\left(\hat{F}^i - \hat{F}^{iL}\right) \qquad \forall t\in TU, i\in t_{out}$$

$$\tilde{F}^i \ge \left(\hat{F}^{iL}\right)^\delta + \left(\frac{\left(\hat{F}^{iU}\right)^\delta - \left(\hat{F}^{iL}\right)^\delta}{\hat{F}^{iU} - \hat{F}^{iL}}\right)\left(\hat{F}^i - \hat{F}^{iL}\right) \qquad \forall i$$

$$\hat{F}^{iL} \le \hat{F}^i \le \hat{F}^{iU}, \ F_n^{iL} \le F_n^i \le F_n^{iU}, \ C_{jn}^{iL} \le C_{jn}^i \le C_{jn}^{iU}$$

$$y^i \in \{0,1\}$$

(CR)

Such a relaxation can be weak when the bounds on the variables are far apart for a large-scale model such as (P), and hence using such relaxations in a branch and bound algorithm slows down the convergence of the algorithm. Tighter relaxations of (P) can alternatively be obtained by extending the concept of Lagrangean decomposition (Guignard and Kim, 1987) to nonconvex MINLP problems. In this work, we combine the concepts of convex relaxations and Lagrangean decomposition to get tight relaxations for model (P). We first construct a Lagrangean relaxation of the original MINLP problem, by dualizing the linking constraints (eq (12)) between the different scenarios. To do this, we create copies of the design variables $\hat{F}^i$ and y^i for each scenario, which are given by $\hat{F}_n^i$ and y_n^i respectively, and replace $\hat{F}^i$ and y^i by these newly created variables in model (P). Hence, eqs (11) and (12) are modified to yield eqs (13) and (14), respectively.

$$\hat{F}^{iL} y_n^i \le \hat{F}_n^i \le \hat{F}^{iU} y_n^i \qquad \forall i, \forall n \in N \tag{13}$$

$$\hat{F}_n^i \ge F_n^i \qquad \forall i, \forall n \in N \tag{14}$$

The objective function is also altered as shown in eq (15) where w_n is a parameter that has to be set so that $\sum_{n=1}^{N} w_n = 1 \qquad 0 \le w_n \le 1$

$$\min z^{RP} = w_n \left[AR\left[\sum_i \left(C_p^i y_n^i + IP^i \left(\hat{F}_n^i\right)^{\delta} \right)\right] + AR \sum_{\substack{t \in TU \\ i \in t_{out}}} IC^t \left(\hat{F}_n^i\right)^{\alpha} \right] + H \sum_n p_n \sum_i PM^i F_n^i + H \sum_n p_n C_{FW} FW_n + H \sum_n p_n \sum_{\substack{t \in TU \\ i \in t_{out}}} OC^t F_n^i \tag{15}$$

Finally, we add eqs (16) and (17) to (P) to obtain a reformulated model (RP).

$$\hat{F}_n^i - \hat{F}_{n+1}^i = 0 \qquad \forall i, \forall n \in N, n < |N| \tag{16}$$

$$y_n^i - y_{n+1}^i = 0 \qquad \forall i, \forall n \in N, n < |N| \tag{17}$$

The equality constraints eq (16) and eq (17) are known as non-anticipativity constraints and require the design variables to be the same in each scenario. Hence, the model (RP) includes the eqs (2) – (10), (13) – (17). Further, we multiply the eqs (16) and (17) with $\lambda_{in}^f \left(\forall n \in N, n < |N|\right)$ and $\lambda_{in}^y \left(\forall n \in N, n < |N|\right)$, respectively, and transfer these constraints to the objective function to get a Lagrangean relaxation of the original problem (P), which is denoted by (LRP) and is decomposable into smaller sub-problems that are easier to solve. The parameters λ_{in}^f and λ_{in}^y are the Lagrange multipliers. The model (LRP) is then decomposed into $|N|$ smaller models that contain variables pertaining to only one scenario. It is to be noted that the bounds of the second stage variables in all the sub-problems are the same as in the original problem, while the bounds of the newly created variables, $\hat{F}_n^i$ and y_n^i are the same as the corresponding design variables $\hat{F}^i$ and y^i, respectively. A set of decomposed problems is as follows:

$$\left.\begin{array}{l}\min z_n = w_n \left[AR\left[\sum_i \left(C_p^i y_n^i + IP^i \left(\hat{F}_n^i\right)^{\delta}\right)\right] + AR \sum_{\substack{t\in TU \\ i\in t_{out}}} IC^t \left(\hat{F}_n^i\right)^{\alpha} \right] + H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n + H\sum_n p_n \sum_{\substack{t\in TU \\ i\in t_{out}}} OC^t F_n^i + \sum_i (\lambda_{in}^f - \lambda_{in-1}^f)\hat{F}_n^i + \sum_i (\lambda_{in}^y - \lambda_{in-1}^y) y_n^i \\ s.t. \quad eqs\,(2)-(10),(13),(14)\end{array}\right\} \quad n = 1,\ldots,|N|$$

where $\lambda_{i0}^f = 0$, $\lambda_{i0}^y = 0$, $\lambda_{i|N|}^y = 0$, $\lambda_{i|N|}^y = 0$ (SP$_n$)

Each of these sub-problems is globally minimized to obtain a solution z_n^*. The sum $z^{LD} = \sum_{n\in N} z_n^*$ yields a valid lower bound to the solution of (P) at a node in the branch and bound tree in a conventional Lagrangean decomposition technique. Such Lagrangean relaxation based lower bounds have been used in a branch and bound setting to solve Mixed Integer Linear Programs (MILPs) by Carøe and Schultz (1999) among other authors. Instead of using such a lower bound we generate valid cuts in the space of the original design and state variables based on the solutions z_n^*, which are given in eq (18).

$$z_n^* \le w_n \left[AR\left[\sum_i \left(C_p^i y^i + IP^i \left(\hat{F}^i\right)^{\delta}\right)\right] + AR \sum_{\substack{t\in TU \\ i\in t_{out}}} IC^t \left(\hat{F}^i\right)^{\alpha} \right] + H\sum_i p_n PM^i F_n^i + H p_n C_{FW} FW_n + H \sum_{\substack{t\in TU \\ i\in t_{out}}} p_n OC^t F_n^i + \sum_i (\lambda_{in}^f - \lambda_{i(n-1)}^f)\hat{F}^i + \sum_i (\lambda_{in}^y - \lambda_{i(n-1)}^y) y^i \qquad n = 1,\ldots,|N|$$

where $\lambda_{i0}^f = 0$, $\lambda_{i0}^y = 0$, $\lambda_{i|N|}^y = 0$, $\lambda_{i|N|}^y = 0$ (18)

In practice we obtain global optimal solutions of nonconvex models with ε_1-tolerance between the lower bounds and the global optimum, so z_n^* is replaced by z_n^{L*} in eq (18), where z_n^{L*} is the highest valued lower bound on the global optimum of sub-problem (SP$_n$). The cuts are valid and do not cut off the global optimum of (P). A proof of the validity of such cuts is given in Karuppiah and Grossmann (2006b). These cuts are then added to the model (P). Futhermore, the Lagrange multipliers can be updated using sub-gradient methods (Fisher, 1985) to derive additional cuts, in the same way as before, to add to the original problem (P) and this procedure of updating the multipliers and adding cuts can be performed any number of times. The initial values of the Lagrange multipliers are chosen arbitrarily. The problem (P) with these cuts added is convexified by constructing convex envelopes for the nonconvex nonlinear terms and the resulting MILP (model (R)) is solved to predict a valid lower bound to the solution of (P) over the sub-region corresponding to a particular node of the search tree. The model (R) (with cuts derived from a single set of Lagrange multipliers) is as follows:

$$\min z^R = AR\left[\sum_i \left(C_p^i y^i + IP^i \widetilde{F}^i\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t \overline{F}^i + H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n \;+\; H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i$$

$$\begin{aligned}
s.t.\quad & F_n^k = \sum_{i\in m_{in}} F_n^i \qquad \forall m\in MU, k\in m_{out}, \forall n\in N\\
& f_{jn}^k = \sum_{i\in m_{in}} f_{jn}^i \quad \forall j, \forall m\in MU, k\in m_{out}, \forall n\in N\\
& F_n^k = \sum_{i\in s_{out}} F_n^i \quad \forall s\in SU, k\in s_{in}, \forall n\in N\\
& C_{jn}^i = C_{jn}^k \qquad \forall j, \forall s\in SU, \forall i\in s_{out}, k\in s_{in}, \forall n\in N\\
& F_n^k = F_n^i = P^p \quad \forall p\in PU, i\in p_{in}, k\in p_{out}, \forall n\in N\\
& P^p C_{jn}^i + L_{jn}^p \times 10^3 = P^p C_{jn}^k \quad \forall j, \forall p\in PU, i\in p_{in}, k\in p_{out}, \forall n\in N\\
& F_n^k = F_n^i \quad \forall t\in TU, i\in t_{out}, k\in t_{in}, \forall n\in N\\
& C_{jn}^i = \beta_{jn}^t C_{jn}^k \quad \forall j, \forall t\in TU, i\in t_{out}, k\in t_{in}, \forall n\in N\\
& \sum_{p\in PU} L_{jn}^p \times 10^3 = \sum_{\substack{t\in TU\\ k\in t_{in}}} \left(1-\beta_{jn}^t\right) f_{jn}^k + f_{jn}^{out} \quad \forall j, \forall n\in N\\
& \hat{F}^{iL} y^i \le \hat{F}^i \le \hat{F}^{iU} y^i \qquad \forall i\\
& \hat{F}^i \ge F_n^i \qquad \forall i, \forall n\in N\\
& \left.\begin{aligned}
f_{jn}^i &\ge F_n^{iL} C_{jn}^i + C_{jn}^{iL} F_n^i - F_n^{iL} C_{jn}^{iL}\\
f_{jn}^i &\ge F_n^{iU} C_{jn}^i + C_{jn}^{iU} F_n^i - F_n^{iU} C_{jn}^{iU}\\
f_{jn}^i &\le F_n^{iL} C_{jn}^i + C_{jn}^{iU} F_n^i - F_n^{iL} C_{jn}^{iU}\\
f_{jn}^i &\le F_n^{iU} C_{jn}^i + C_{jn}^{iL} F_n^i - F_n^{iU} C_{jn}^{iL}
\end{aligned}\right\} \quad \forall j, \forall m\in MU, \forall i\in\{m_{in}\cup m_{out}\}, \forall n\in N\\
& \overline{F}^i \ge \left(\hat{F}^{iL}\right)^{\alpha} + \left(\frac{\left(\hat{F}^{iU}\right)^{\alpha} - \left(\hat{F}^{iL}\right)^{\alpha}}{\hat{F}^{iU} - \hat{F}^{iL}}\right)\left(\hat{F}^i - \hat{F}^{iL}\right) \qquad \forall t\in TU, i\in t_{out}\\
& \widetilde{F}^i \ge \left(\hat{F}^{iL}\right)^{\delta} + \left(\frac{\left(\hat{F}^{iU}\right)^{\delta} - \left(\hat{F}^{iL}\right)^{\delta}}{\hat{F}^{iU} - \hat{F}^{iL}}\right)\left(\hat{F}^i - \hat{F}^{iL}\right) \qquad \forall i\\
& z_n^* \le w_n\left[AR\left[\sum_i \left(C_p^i y^i + IP^i \widetilde{F}^i\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t \overline{F}^i\right] + H\sum_i p_n PM^i F_n^i + Hp_n C_{FW} FW_n \;+\; H\sum_{\substack{t\in TU\\ i\in t_{out}}} p_n OC^t F_n^i + \sum_i (\lambda_{in}^f - \lambda_{i(n-1)}^f)\hat{F}^i + \sum_i (\lambda_{in}^y - \lambda_{i(n-1)}^y) y^i \qquad n=1,\ldots,|N|\\
& \hat{F}^{iL} \le \hat{F}^i \le \hat{F}^{iU}, F_n^{iL} \le F_n^i \le F_n^{iU}, C_{jn}^{iL} \le C_{jn}^i \le C_{jn}^{iU}\\
& y^i \in \{0,1\}
\end{aligned}$$

(R)

The lower bound obtained by solving (R) is at least as strong as the lower bound obtained by model (CR) since the feasible region of model (R) is more constrained than the feasible region of (CR) since it includes the Lagrangean based cutting planes. Also, the lower bound obtained by solving (R) would be at least as strong as the lower bound obtained from a conventional Lagrangean decomposition method. This is because if we take a sum over all n $\in N$, of the left and right hand sides of the cuts included in model (R), we get the following result:

$$z^{LD} = \sum_{n\in N} z_n^* \le AR\left[\sum_i \left(C_p^i y^i + IP^i \widetilde{F}^i\right)\right] + AR\sum_{\substack{t\in TU\\ i\in t_{out}}} IC^t \overline{F}^i + H\sum_n p_n \sum_i PM^i F_n^i + H\sum_n p_n C_{FW} FW_n \;+\; H\sum_n p_n \sum_{\substack{t\in TU\\ i\in t_{out}}} OC^t F_n^i$$

The right hand side in the above expression is the objective function of model (R) and so on solving (R), we would get an objective value greater than or equal to $\sum_{n \in N} z_n^*$. It should be noted that solving (R) can sometimes be computationally expensive, but the tighter lower bounds obtained on solving (R) can help in accelerating the convergence of the branch and bound algorithm.

Remarks:

(i) It is not necessary to solve $|N|$ global optimization problems at every node of the tree, as is required in a pure Lagrangean decomposition based algorithm to obtain a valid lower bound. Any number of cuts can be generated as decided by the user and included in the relaxation to get strong lower bounds.

(ii) It is not required that the model (P) be decomposed into |N| sub-models, since the Lagrangean relaxation (LRP) can be decomposed into N′ (< |N|) models if some of the non-anticipativity constraints are not relaxed.

(iii) There are multiple ways to decompose model (LRP) by assigning different values to the parameter w_n. The cuts derived from using different values of w_n are all valid and can be added simultaneously to (P) which can help in further tightening the relaxation (R).

4.2. Upper bound generation: A heuristic procedure is used to generate upper bounds at every node of the branch and bound tree. We solve the relaxation (R) and obtain a integer solutions to the binary variables y^i in (P). We fix the binary variables in (P) to the corresponding values obtained by solving the relaxation (R), and optimize the resulting nonconvex NLP model using the optimal values of the continuous variables obtained by solving (R) as starting points. The optimal objective value of this nonconvex NLP model thus found serves as an upper bound on the global optimum of (P). Alternatively, a locally optimal solution to (P) can be found using a local solver such as DICOPT, which serves as an upper bound.

4.3. Spatial Branch and Cut algorithm:

The proposed algorithm is summarized as follows:

1. Pre-processing The numerical data for the integrated water network that includes the water demands in the process units, the inlet concentration restrictions on the contaminants entering

these units, the discharge concentration limits, and the values of the uncertain parameters in different scenarios, is used to determine the bounds on the variables in the model. The bounds on the design variables $\hat{F}^i$ are chosen such that the bounds on the flows F_n^i in each scenario *n*, lie between the design variable bounds, that is, $\hat{F}^{iL} \le F_n^{iL} \le F_n^{iU} \le \hat{F}^{iU}$, where $\hat{F}^{iL}$ and $\hat{F}^{iU}$ are the design variable bounds and F_n^{iL} and F_n^{iU} are the bounds on the flows in scenario *n*. Further in this step, the nonconvex MINLP may be locally optimized to get an initial overall upper bound (z^{OUB}) on the objective function.

2. Obtaining Lower bounds At every node of the search tree, this step includes the following:

(a) Construct a Lagrangean relaxation of (P) and get model (LRP), decomposing it into |N| scenarios to obtain sub-problems (SP_1) – ($SP_{|N|}$).

(b) Solve each sub-problem (SP_n) n=1, …, |N|, to global optimality (within ε_1-tolerance) using any deterministic global optimization technique to get solutions $z_n^* \quad \forall n$. Let z_n^{L*} be the highest possible lower bound on z_n^*, where $(1-\varepsilon_1)z_n^* \le z_n^{L*} \le z_n^*$. If the optimal values of the variables $\hat{F}_n^{i*}$ and y_n^{i*}, obtained from solving the sub-problems, are feasible for model (RP), then we can fathom the node and go to step 5. Prior to fathoming the node, we check if $\sum_n z_n^* \le z^{OUB}$, and if so, we set $z^{OUB} = \sum_n z_n^*$. If any of the sub-problems (SP_n) n=1, …, |N| is found to be infeasible, the node is fathomed. The model (P) is infeasible if this occurs at the root node to the tree.

(c) From the global optima of the sub-problems, derive the cuts in eq (18). Note that z_n^{L*} should be used in the equations for the cutting planes. Update the Lagrange multipliers to generate more cuts.

(d) Add all derived cuts to (P) to get model (P'), whose MILP relaxation (R) is solved to obtain a rigorous lower bound (z^R) on the solution at a node. If at a certain node, the model (R) is found to be infeasible, the node is fathomed from the tree.

3. Upper bounding problem An upper bound or locally optimal solution to the original MINLP is obtained using the heuristic procedure given in section 4.2, and if there is an improvement with respect to the z^{OUB}, it is updated.

4. Termination of search A node in the tree is fathomed if either the lower bound at the node is greater than z^{OUB}, or if the relaxation gap between the lower and overall upper bound is lesser than a certain tolerance. The relaxation gap at any node in the tree is defined as:

$$relaxation\ gap = \begin{cases} \left| \dfrac{z^{OUB} - z^{R}}{z^{OUB}} \right| & if\ z^{OUB} \neq 0 \\ -z^{R} & if\ z^{OUB} = 0 \end{cases}$$

The absence of any open nodes in the tree calls for stopping the search.

5. Spatial branch and bound Regions of the search space for which the relaxation gap is greater than the specified tolerance are further partitioned into disjoint sub-regions to create new nodes in the tree and steps 2 – 4 are repeated for each of these regions. The convex envelope equations along with the duality based cuts in the lower bounding problem are updated in each newly created partition, thus yielding tighter lower bounds in nodes down the tree. The branching down the tree is based on some heuristics. The design variables $\hat{F}^{i}$ and y^{i} are used as the branching variables. If the duplicate variables corresponding to a design variable take the same value in the solution of all the sub-problems at a node of the tree for a particular set of Lagrange multipliers, then the corresponding design variable is not chosen as the branching variable. The dispersion of a design variable $\hat{F}^{i}$ is defined as $\sum_{n} \dfrac{\left| \hat{F}_{n}^{i*} - F_{av}^{i} \right|}{\left| \max_{n}\{\hat{F}_{n}^{i*}\} - \min_{n}\{\hat{F}_{n}^{i*}\} \right|}$, where $\hat{F}_{n}^{i*}$ is the optimal value of the duplicate variable corresponding to $\hat{F}^{i}$ in the nth sub-problem (SP_n), and $F_{av}^{i} = \dfrac{\sum_{n} \hat{F}_{n}^{i*}}{|N|}$. The dispersion of a binary variable y^{i} is similarly defined. The dispersion of all the design variables is computed for every set of Lagrange multipliers that is used to derive the Lagrangean cuts, and the design variable with the maximum dispersion is chosen as the branching variable. If $\hat{F}^{i}$ is chosen as the branching variable, then F_{av}^{i} is taken as the branching point. In case y^{i} is chosen as the branching variable, we create two new branches corresponding to $y^{i} = 1$ and $y^{i} = 0$. A depth first strategy is used to traverse the tree.

Convergence: Spatial branch and bound is theoretically an infinite process since branching is performed on continuous variables, but it terminates in a finite number of steps for εconvergence. In this algorithm, the search region is successively partitioned into disjoint sub-regions, where the lower and upper bounding problems are solved. This kind of partitioning and narrowing the search region yields a sequence of tighter relaxations and non-decreasing lower bounds down the search tree, which guarantees convergence of the branch and bound algorithm (Horst and Tuy, 1996).

Remarks

(i) This algorithm can easily be parallelized and the sub-problems can be solved in parallel to reduce the computational expense.

(ii) The model (P') (with the cuts added) can be solved using commercial MINLP solvers (e.g. BARON) in reduced times.

5. NUMERICAL EXAMPLES

Two illustrative examples of the integrated water networks operating under uncertainty were solved using the proposed algorithm. The multiscenario MINLP models correspodning to the examples were formulated using GAMS (Brooke et al., 1998) and solved on an Intel 3.2 GHz Linux machine with 1024 MB memory. GAMS/CONOPT 3.0 was used to solve the NLP problems, GAMS/CPLEX 9.0 was used for the MILP problems, and GAMS/DICOPT and GAMS/ BARON 7.2.5 were employed for solving the MINLP problems.

Example 1 As a first example, we consider a network consisting of two water processing units and two water treatment units whose superstructure is shown in Fig. 1. It is a system involving two contaminants A and B which are generated in the process units and removed using the treatment units. The concentration of these pollutants has to be reduced to less than 10 ppm in the effluent stream discharged into the environment. This system operates over a set of 10 scenarios, where the operational conditions are different in each scenario. The model developed for representing the integrated network is optimized using the process unit data and treatment unit data given in tables 1 and 2 respectively. The probabilities corresponding to each scenario are given in table 3.

Table 1. Process unit data for example 1

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	Maximum Inlet Conc. (ppm) A	B
PU1	40	A	2	1	0.5	1	1	2	0.5	1	0.5	2	0	0
		B	2.5	1.5	1	1.5	1.5	2.5	1	1.5	1	2.5		
PU2	50	A	2	1	0.5	2	1	1	1	0.5	2	0.5	50	50
		B	2	1	0.5	2	1	1	1	0.5	2	0.5		

Table 2. Treatment unit data for example 1

Unit	Removal ratio (%)	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10	IC ($)	OC ($/ton)	α
TU1	A	90	95	99	95	99	95	95	99	95	90	16800	1	0.7
	B	0	0	0	0	0	0	0	0	0	0			
TU2	A	0	0	0	0	0	0	0	0	0	0	12600	0.0067	0.7
	B	90	95	99	95	95	95	90	90	95	95			

Table 3. Probabilities corresponding to each scenario for example 1

Scenario	n1	n2	n3	n4	n5	n6	n7	n8	n9	n10
Probability	0.2	0.3	0.15	0.1	0.05	0.05	0.03	0.02	0.05	0.05

Additionally, the following data is required for the optimization: the cost of freshwater is assumed to be $1/ ton, the annualized factor for investment taken to be 0.1, the cost coefficients pertaining to the pipes is taken as $ 6 while the investment cost coefficient for each individual pipe is assumed to be $ 100 and operating cost coefficients for pumping water in the pipes is taken as $ 0.006 / ton. The network is continuously operated for 8000 hours in a year. This multiscenario MINLP corresponding to this example involves 24 binary variables, 764 continuous variables, 928 constraints and 406 nonconvex terms. On directly using BARON to solve the problem, the solver could not verify global optimality to required tolerance of 1 % in more than 10 hours.

The application of the proposed algorithm yields an expected total cost of $ 651,653.06 / yr (first stage annualized capital cost = $ 46,189.93 /yr; second stage expected operating cost = $ 605,463.13 /yr) , which is the global solution to the problem. It is also found that the lower and upper bounds converge to within the specified tolerance at the root node of the branch and bound tree.

Application of algorithm to example 1: An overall upper bound is initially found by solving the original nonconvex MINLP model using DICOPT which yielded a local optimum of \$685,466.48. The Lagrangean relaxation of the original model is then formulated and decomposed into 10 different sub-problems (each sub-problem corresponding to one scenario) as described in section 4.1. With the initial values of all the Lagrange multipliers taken to be 1, each of these sub-problems is solved to global optimality with 1 % tolerance for the gap between the lower and upper bounds. Next, we substitute the best valid lower bounds obtained from the solution of each sub-problem into z_n^* in eq (18) to generate 10 valid cuts. The Lagrange multipliers are then updated to generate 10 more valid cutting planes. We add these 20 cuts to the original nonconvex MINLP model and the problem is then convexified to yield a MILP relaxation (R), which when solved to optimality provides a lower bound of \$ 645,948.7. At the root node, we find an upper bound of \$ 651,653.06 using the heuristic in section 4.2. Thus, the lower and upper bounds lie within the tolerance of 1% at the root node. The relaxation gap between the lower and upper bounds is further reduced to within 0.5 % by branching down the tree on a continuous design variable (see Table 4 for details). Table 4 shows that the lower bound obtained using the proposed technique, at every node of the search tree, is stronger than the ones obtained from a MILP relaxation of (P) (model (CR)), and from a conventional Lagrangean decomposition technique.

Table 4. Numerical results for example 1

Node #	Lower bound using proposed algorithm (z^R)	Best bound from Lagrangean Decomposition (z^{LB})	Lower bound from MILP Relaxation (z^{CR})	Upper Bound (z^{UB})	Total time taken at node[†] (CPUsecs)
0 (root node)	**645,951.64**	644,856.82	610,092.61	651,653.65	19.33
1	**648,566.716**	647,496.24	610,115.37	672,971.83	4.1
2	**648,828.60**	648,073.24	610,109.06	661,439.35	61.83

The total time taken for finding the global optimum using the proposed algorithm is 85.56 CPUsecs, which includes the time for getting an initial overall upper bound using DICOPT. The optimal network topology is shown in Fig. 2 where, alongside the pipe connections, the maximum flowrates that can be handled by the pipes are shown.

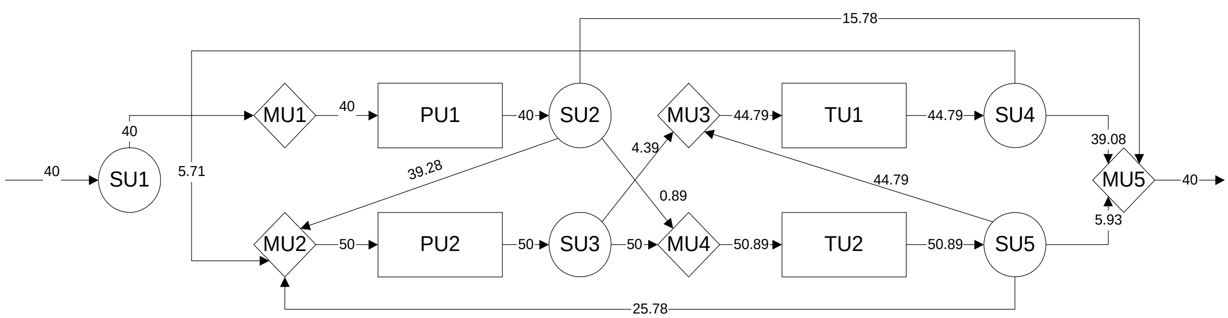

Fig. 2 Global optimal solution for water network with 2 Process Units – 2 Treatment Units operating under uncertainty

Robustness of Design It can be proved that when the network is designed for the worst-case scenario, that is, with the highest contaminant loads in the process units and the lowest contaminant removals in the treatment units, the design is robust. This means that this particular network design is such that the network can be operated feasibly for all cases where the contaminant loads in the process units are lower and the contaminant removals in the treatment units are higher. It is trivial to prove the above using the following analysis:

[†] Total time includes time for generating cuts, solving the master problem and generating an upper bound

Let us look at the example of two process unit – two treatment unit network, that has been designed for the worst-case scenario (Fig. 3) using the data given in Tables 5 and 6 and the previous cost information. The model is a single scenario model with the probability of its occurrence set to 1.

Table 5. Process unit data for worst-case scenario

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr) A	B	Maximum Inlet Concentration (ppm) A	B
PU1	40	2	2.5	0	0
PU2	50	2	2	50	50

Table 6. Treatment unit data for worst-case scenario

Unit	Removal ratio (%) A	B	IC ($)	OC ($/ton)	α
TU1	90	0	16800	1	0.7
TU2	0	90	12600	0.0067	0.7

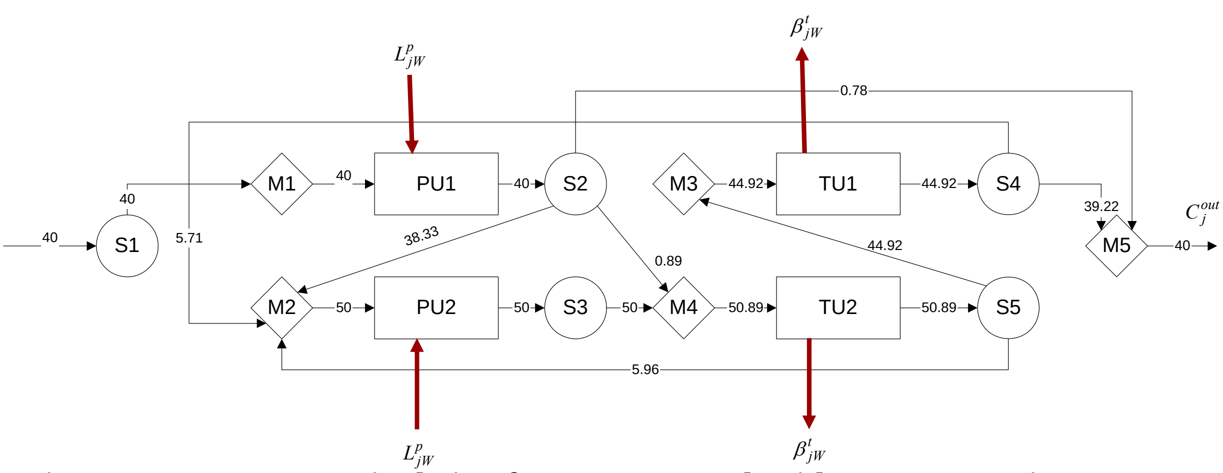

Fig. 3 Worst-case scenario design for water network with 2 Process Units – 2 Treatment Units

The demands in the process units have to be met over each different scenario. The contaminant levels in the streams inlet to the process units and in the discharge out to the environment have fall below specified limits. The worst-case design corresponds to the highest contaminant loads in the process units (L^p_{jW}) and the lowest contaminant removals in the treatment units (this corresponds to the highest β_j^t, given by β_{jW}^t). Let us now say that the operating flows (control variables) remain the same as for the worst case, in all the scenarios $n \in$ N. In all the scenarios apart from the worst case, the contaminant loads entering the water streams in the network are lower and the contaminant removals in the treatment units are higher, that is $L_{jn}^p \le L_{jW}^p \;\; \forall n$ and $\beta_{jn}^t \le \beta_{jW}^t \;\; \forall n$. Since the water flows through the network are not changing, the concentration of contaminants in every stream in the network can only decrease since the concentration is given by : Contaminant amount in a stream/ Flow in a stream. Hence, assuming that the inlet concentrations to the process units are not higher than the worst-case scenario in any scenario, the contaminant concentrations in the streams exiting the process units (PU1 -> SU2, PU2 -> SU3) and in the streams exiting the treatment units (TU1 -> SU4, TU2 -> SU5) are lower than the concentrations in the worst-case scenario. The contaminant concentrations of the streams leaving the splitters (SU2, SU3, SU4, SU5) are equal to the concentrations entering these splitters, and hence lower than the corresponding concentrations in the worst-case scenario. Since these splitters direct water to the inlet of the process units and also the discharge to the environment, a combination of the contaminant concentrations in these streams cannot lead to concentrations that exceed the worst-case scenario levels at the inlet to the process units and in the discharge to the environment.

Hence, if the worst-case design is used and the worst-case operating flows are used in every scenario, the network operation will still be feasible in every scenario in terms of the contaminant concentration constraints that have to be met.

To see how the worst-case design compares to the previous design, we calculate the design cost of integrated network designed for the worst-case scenario, and the expected cost of operating it over 10 scenarios. The first stage annualized design cost for this system is $ 46,051.60 /yr. This design, shown in Fig. 3, is still operated over 10 scenarios and so the second stage expected operating costs for this network, are $ 714,639.58 /yr, and hence the total cost for this network is $ 760,691.18 /yr. The expected operating cost is much higher for this design as compared to the previous design (Fig. 2), since the new design has one less pipeline and hence some of the flexibility of operating the network is lost, leading to the increased operating cost.

If we instead globally optimize the system considering three scenarios, where the values of the uncertain parameters can be classified as - ‘low’ , ‘normal’ and ‘high’, we obtain a different network design (see Fig. 4). The term ‘low’ corresponds to the case when the contaminant loads in the process units are at their lowest values and the contaminant removals in the treatment units are at their highest values (that is, best-case). The scenario with ‘normal’ values of the uncertain parameters is the base case when the uncertain parameters take on their nominal values, and finally, the term ‘high’ is used to denote the case when the contaminant loads take their maximum values and the contaminant removals are their lowest (i.e., worst-case). The relevant cost data for the optimization is the same as given at the start of this example, while the numerical data for the optimization is given in Tables 7, 8 and 9. Note that nearly equal probabilities are assumed for each scenario. The MINLP for this case involved 24 binary variables, 314 continuous variables, and 380 constraints and using the proposed algorithm, the global solution is obtained in 7.6 CPUsecs.

Table 7. Process unit data for three scenario case

Unit	Flowrate (ton/hr)		Discharge load (Kg/hr) n1	n2	n3	Maximum Inlet Conc. (ppm) A	B
PU1	40	A	2	1	0.5	0	0
		B	2.5	1.5	1		
PU2	50	A	2	1	0.5	50	50
		B	2	1	0.5		

Table 8. Treatment unit data for three scenario case

Unit		Removal ratio (%) n1	n2	n3	IC ($)	OC ($/ton)	α
TU1	A	90	95	99	16800	1	0.7
	B	0	0	0			
TU2	A	0	0	0	12600	0.0067	0.7
	B	90	95	99			

Table 9. Probabilities corresponding to each scenario in the three scenario case

Scenario	n1	n2	n3
Probability	0.33	0.34	0.33

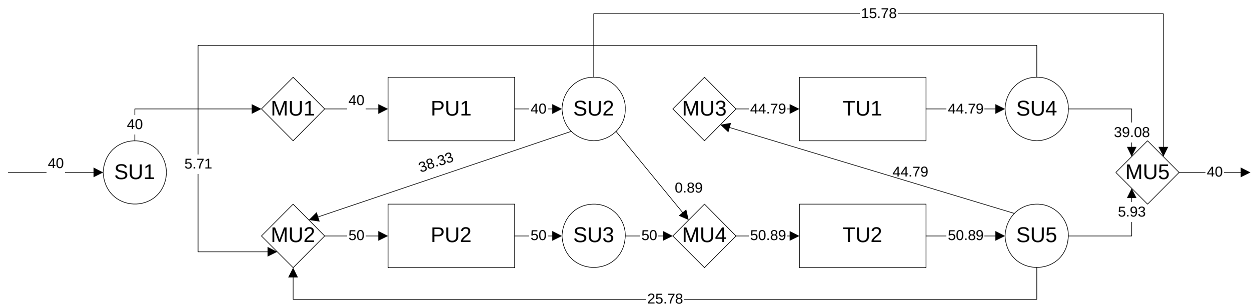

Fig. 4 Globally optimal network design for water network with 2 Process Units – 2 Treatment Units operating under 3 scenarios

The design in Fig. 4 is closer to the one in Fig. 2, and its annualized design cost is $ 46,158.96 /yr, and its expected operating cost (over the initial 10 scenarios) is $ 605,538.16 /yr. The total cost of this network is $ 651,697.12 /yr, which is very close to the total cost of Fig. 1. Hence, the design of the network with 3 scenarios (low, normal and high) is a good approximation of the network design with 10 scenarios.

Example 2 As a second example, we optimize a larger system with 5 process units and 3 treatment units that involves 3 contaminants (A, B and C). The uncertainty in the contaminant loads and contaminant removals is represented using 3 scenarios. The numerical data for the optimization is given below:

Table 10. Process unit data for example 2

Unit	Flowrate (ton/hr)	Discharge load (Kg/hr)				Maximum Inlet Conc. (ppm)		
			n1	n2	n3	A	B	C
PU1	40	A	1	1.5	2	0	0	0
		B	1.5	2	2.5			
		C	1	1.5	2			
PU2	50	A	1	1.5	2	50	50	50
		B	1	1.5	2			
		C	1	1.5	2			
PU3	60	A	1	1.5	2	50	50	50
		B	1	1.5	2			
		C	1	1.5	2			
PU4	70	A	2	2.5	3	50	50	50
		B	2	2.5	3			
		C	2	2.5	3			
PU5	80	A	1	1.5	2	25	25	25
		B	1	1.5	2			
		C	0	0.5	1			

Table 11. Treatment unit data for example 2

Unit		Removal ratio (%) n1	n2	n3	IC ($)	OC ($/ton)	α
TU1	A	95	96	94	16800	1	0.7
	B	0	0	0			
	C	0	0	0			
TU2	A	0	0	0	9500	0.04	0.7
	B	0	0	0			
	C	95	96	94			
TU3	A	0	0	0	12600	0.0067	0.7
	B	95	96	94			
	C	0	0	0			

Table 12. Probabilities corresponding to each scenario for example 2

Scenario	n1	n2	n3
Probability	0.33	0.34	0.33

The other relevant numerical data for the optimization is the same as in example 1. The MINLP model corresponding to this example had 77 binary variables, 1222 continuous variables and 1377 constraints. The global optimization solver BARON found a solution of $1,535,648.88 /yr and a lower bound of $ 1,346,129.19 /yr (14 % relaxation gap) after 11 CPUhours of computation. Using the proposed algorithm, we find the global solution of $ 1,369,067.5 /yr and a lower bound of $ 1,347,297.36 /yr, at the root node of the search tree and terminate the search there. The total time taken was 193.48 CPUsecs. The optimal network structure is shown in Fig.5.

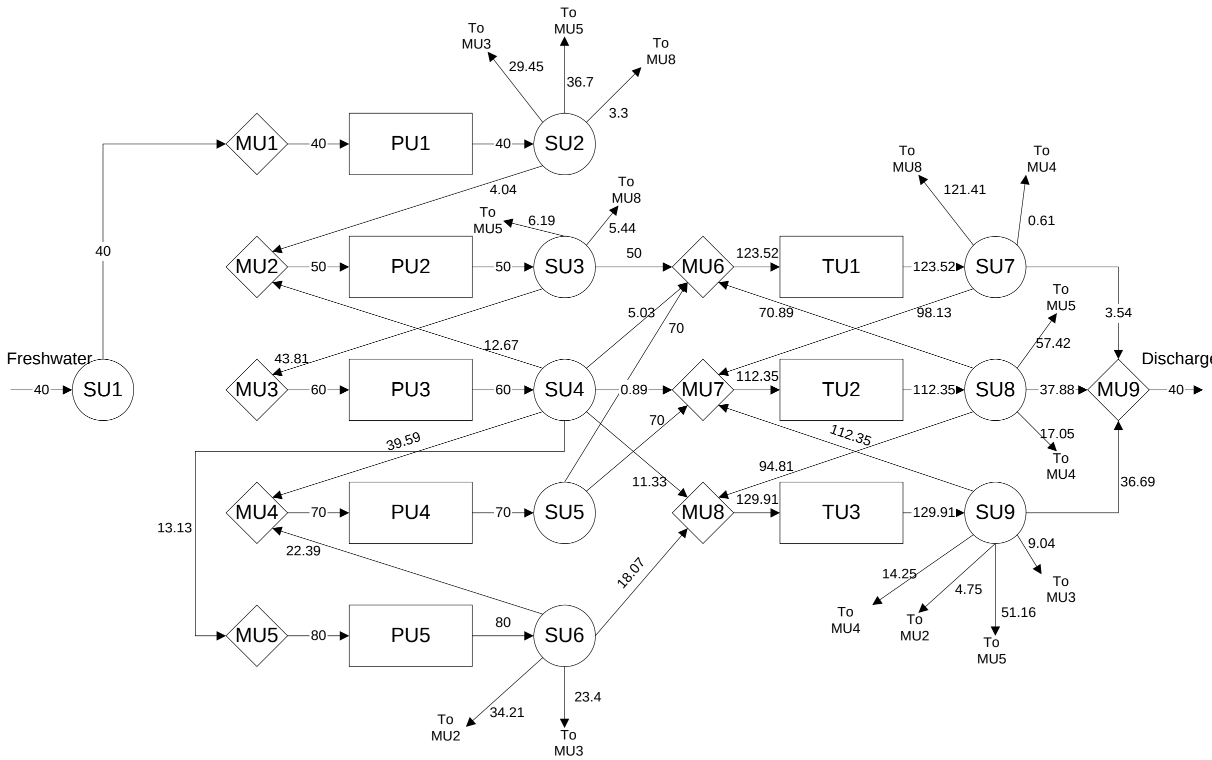

Fig. 5 Global optimal solution for water network with 5 Process Units – 3 Treatment Units operating under uncertainty

6. CONCLUSIONS

In this work, we have presented a formulation for representing and optimizing integrated water networks operating under uncertain conditions in the process industry. The uncertainties are in contaminant loads in the process units and the contaminant removals inside the treatment units. The uncertainty in the system is characterized through the use of scenarios, where the uncertain parameters take on different values.

A multiscenario noncovex MINLP model was formulated to globally optimize an integrated water network operating under uncertainty. To solve such large scale models to global optimality, we have proposed a special branch and cut algorithm. This algorithm involves decomposing the original model into different scenarios based on Lagrangean duality and generating valid cuts based on the global solutions of each of the smaller sub-problems. We add these cuts to the original nonconvex MINLP model and convexify the resulting model to get a MILP relaxation whose solution provides a tight lower bound on the solution at every node of the branch and cut tree. The novelty of this algorithm lies in combining the concepts of Lagrangean relaxation and convex relaxations in order to generate strong bounds on the global optimum of the nonconvex MINLP model. The algorithm was applied to two integrated water systems involving uncertainty in their operational conditions. The solution times are reduced by more than an order of magnitude as compared to a commercial global optimization solver, on applying the proposed technique on these examples illustrating the efficacy of the algorithm in solving such large scale models.

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Nomenclature

Sets and Indices

i,k	stream indices
j	contaminant
m	mixer
m_{in}	set of inlet streams into mixer m
m_{out}	outlet stream from mixer m
MU	set of mixers
n	scenario
N	set of scenarios
p	process unit
p_{in}	inlet stream into process unit p
p_{out}	outlet stream from process unit p
PU	set of process units
s	splitter
s_{in}	inlet stream into splitter s
s_{out}	set of outlet streams from splitter s
SU	set of splitters

t treatment unit

t_{in} inlet stream into treatment unit t

t_{out} outlet stream from treatment unit t

TU set of treatment units

Parameters

α cost function exponent ($0 < \alpha \le 1$)

δ cost function exponent ($0 < \delta \le 1$)

β_{jn}^{t} 1 – {(Removal ratio for contaminant j in unit t (in %)) in scenario n/ 100}

$\lambda_{in}^{f}, \lambda_{in}^{y}$ Lagrange multipliers

AR annualized factor for investment on treatment units

C_{FW} cost of freshwater

C_p^i cost coefficient corresponding to existence of pipe i

C_{jn}^{iL} lower bound on concentration of contaminant j in stream i in scenario n

C_j^{iU} upper bound on concentration of contaminant j in stream i in scenario n

F_n^{iL} lower bound on flow in stream i in scenario n

F_n^{iU} upper bound on flow in stream i in scenario n

$\hat{F}^{iL}$ lower bound on design variable $\hat{F}^i$

$\hat{F}^{iU}$ upper bound on design variable $\hat{F}^i$

H hours of plant operation per annum

IC^t investment cost coefficient for treatment unit t

IP^i investment cost coefficient for pipe i

L_{jn}^{p} load of contaminant j inside process unit p in scenario n

OC^t operating cost coefficient for treatment unit t

PM^i operating cost coefficient for pumping water through pipe i

P^p flow demand in process unit p

Continuous Variables

C^{i}_{jn} concentration of contaminant *j* in stream *i* in scenario *n*

$\hat{F}^{i}$ maximum flow of water allowed in pipe *i*

f^{i}_{jn} flow of contaminant *j* in stream *i* in scenario *n*

f^{out}_{jn} flow of contaminant *j* in the outlet stream to the environment in scenario *n*

F^{i}_{n} flowrate of stream *i* in scenario *n*

FW_n freshwater intake into the system in scenario *n*

Binary variables

y^{i} equal to 1 if pipe *i* exists in the network

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