

Global Optimization of Water Management Problems Using Linear Relaxation and Bound Contraction Methods

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ABSTRACT: In this paper, we present results of a recently developed global optimization method¹ as applied to water management problems. Our method deals effectively with MINLP problems with bilinear and univariate concave terms. Bilinear terms show up in these problems as products of flow rates and concentrations in component balances. In turn, concave terms are typically associated with equipment costs.

1. INTRODUCTION

Several methods have been presented to obtain globally optimal solution of water problems: Karupiah and Grossmann² use a deterministic spatial branch and contract algorithm, in which the bilinear terms are relaxed using the convex and concave envelopes³ and the concave terms of the objective function are replaced by underestimators generated by the secant of the concave term. The model is solved using disjunctions and a spatial branch and bound contraction procedure, which is a simplified version of the one used by Zamora and Grossmann.⁴ Later, Karupiah and Grossmann⁵ extended their method to solve integrated water systems using a spatial branch and cut algorithm that uses Lagrangean relaxation. Bergamini et al.⁶ proposed an outer approximation method (OA) for global optimization. Bergamini et al.⁷ introduced underestimators (which replace the concave and bilinear terms) using the delta-method of piecewise functions.⁸ They also replace the global solution of the bounding problem by a strategy based on the mathematical structure of the problem, which searches for better feasible solutions of fixed network structures. Subproblems need to be solved to feasibility instead to optimality.

Meyer and Floudas⁹ proposed a piece-wise reformulation-linearization technique (RLT) for wastewater treatment systems, which they treat as a generalized pooling problem. They partition the continuous space of one of the variables participating in a bilinear term in several intervals to generate a MINLP, allowing them to linearize the model to be able to generate lower bounds.

In a recent paper,¹ we made a more thorough revision of the global optimization-related literature corresponding to water problems and proposed a new method to obtain the global optimum of MINLP problems with bilinear and univariate concave terms. The procedure we proposed consists of constructing an MILP lower bound based on partitioning the feasible space of certain variables and allow a relaxation of the bilinear terms. Instead of resorting to a branch and bound strategy like the one employed by other procedures, we perform a set of bound contraction steps, which are based on an interval elimination procedure. In this paper, we present the results of our method, and we compare them with results obtained using other global optimization procedures.

The paper is organized as follows: We present the solution strategy first, followed by examples for water management problems and finally for pooling and generalized pooling problems.

2. SOLUTION STRATEGY

We define different variables: *partitioning variables*, which are the ones that generate several intervals and are used to construct linear relaxations of bilinear term, *bound contracted variables*, which are also partitioned into intervals, but only for the purpose of performing their bound contraction, and *branch and bound variables*, which are the variables for which a branch and bound procedure is tried. Although the bound contract variable and branch and bound variable do not need to be the same as the partitioned one, it is normal to have them being bound contracted or branched, as opposed to picking other variables. In some cases, picking the variable to bound contract different from the one to partition renders tighter lower bounds as bound contraction takes place.

After partitioning one of the variables in the bilinear terms, our method consists of a bound contraction step that uses a procedure for eliminating intervals. Once the bound contraction is exhausted, the method relies on increasing the number of intervals or on a branch and bound strategy, where the interval elimination takes place at each node. The partitioning methodology generates linear models that guarantee to be lower bounds of the problem. Upper bounds are needed for the bound contraction procedure. These upper bounds are usually obtained using the original MINLP model often initialized by the results of the lower bound model.

The global optimization strategy is now summarized as follows:

- Construct a lower bound model partitioning variables in bilinear and quadratic terms, to relax the bilinear terms as well as adding piece-wise linear underestimators of concave terms of the objective function.
- The lower bound model is run identifying certain intervals as containing the solution for specific variables.

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- Obtain an upper bound by running the original MINLP using the information obtained by solving the lower bound model.
- A strategy based on the successive running of lower bounds follows: Here, certain intervals are temporarily forbidden and the results of the relaxed model are used as guidance to eliminate regions of the feasible space. In essence when a certain interval is forbidden and the relaxed model renders an objective larger than the current upper bound value, then the forbidden interval is the only one surviving and the rest are eliminated. This is the bound contraction part.
- The process is repeated with new bounds until convergence or until the bounds cannot be contracted anymore.
- If the bound contraction is exhausted, there are two possibilities to guarantee global optimality: increase partitioning or split the problem in two and start a branch and bound procedure.
- Convergence is achieved when upper and lower bounds differ by some small gap.

3. WATER MANAGEMENT MODEL

The optimization of water systems can be stated as follows: *Given sets of water using units, freshwater source and potential regeneration processes (water pretreatment and/or wastewater treatment units), one wants to obtain a water/wastewater network that globally optimizes a chosen objective function.*

The above problem statement has different forms depending on the level of detail of the model and the nature of the objective function. In its simplest form, the most popular objective function is the freshwater consumption.

Several other models have been proposed for water systems with different cost objectives,^{2,10–14} forbidden matches,^{10,14} costing of regeneration units,^{2,13,14} and profitability.^{15–20}

Aside from the differences in the objective functions, architectural or modeling assumptions can also change the problem statement. More details can be found in a recent paper,²¹ where these issues are discussed.

The model we use to optimize the water systems is given by the following constraints and objective function:

Water Balance at the Water-Using Units.

$$\sum_w \text{FWU}_{w,u} + \sum_{u^* \neq u} \text{FUU}_{u^*,u} + \sum_r \text{FRU}_{r,u} = \sum_s \text{FUS}_{u,s} + \sum_{u^* \neq u} \text{FUU}_{u,u^*} + \sum_r \text{FUR}_{u,r} \quad \forall u \quad (1)$$

where $\text{FWU}_{w,u}$ is the flow rate from freshwater source w to the unit u , $\text{FUU}_{u^*,u}$ is the flow rates between units u^* and u , $\text{FRU}_{r,u}$ is the flow rate from regeneration process r to unit u , $\text{FUS}_{u,s}$ is the flow rate from unit u to sink s and $\text{FUR}_{u^*,y}$ is the flow rate from unit u to regeneration process r .

Water Balance at the Regeneration Processes.

$$\sum_w \text{FWR}_{w,r} + \sum_u \text{FUR}_{u,r} + \sum_{r^*} \text{FRR}_{r^*,r} = \sum_u \text{FRU}_{r,u} + \sum_{r^*} \text{FRR}_{r,r^*} + \sum_s \text{FRS}_{r,s} \quad \forall r \quad (2)$$

where $\text{FWR}_{w,r}$ is the flow rate from freshwater source w to the regeneration process r , $\text{FRR}_{r^*,r}$ is the flow rate from regeneration process r^* to regeneration process r and $\text{FRS}_{r,s}$ is the flow rate from regeneration process r to sink s .

Contaminant Balance at the Water-Using Units.

$$\sum_w (\text{CW}_{w,c} \text{FWU}_{w,u}) + \sum_{u^* \neq u} \text{ZUU}_{u^*,u,c} + \sum_r \text{ZRU}_{r,u,c} + \Delta M_{u,c} = \sum_{u^* \neq u} \text{ZUU}_{u,u^*,c} + \sum_s \text{ZUS}_{u,s,c} + \sum_r \text{ZUR}_{u,r,c} \quad \forall u, c \quad (3)$$

where $\text{CW}_{w,c}$ is concentration of contaminant c in the freshwater source w , $\Delta M_{u,c}$ is the mass load of contaminant c extracted in unit u , $\text{ZUU}_{u^*,u,c}$ is the mass flow of contaminant c in the stream leaving unit u^* and going to unit u , $\text{ZRU}_{r,u,c}$ is the mass flow of contaminant c in the stream leaving regeneration process r and going to unit u , $\text{ZUS}_{u,s,c}$ is the mass flow of contaminant c in the stream leaving unit u and going to sink s , and $\text{ZUR}_{u,r,c}$ is the mass flow of contaminant c in the stream leaving unit u and going to regeneration process r .

Maximum Inlet Concentration at the Water-Using Units.

$$\sum_w (\text{CW}_{w,c} \text{FWU}_{w,u}) + \sum_{u^* \neq u} \text{ZUU}_{u^*,u,c} + \sum_r \text{ZRU}_{r,u,c} \leq C_{u,c}^{\text{in,max}} (\sum_w \text{FWU}_{w,u} + \sum_{u^* \neq u} \text{FUU}_{u^*,u} + \sum_r \text{FRU}_{r,u}) \quad \forall u, c \quad (4)$$

where $C_{u,c}^{\text{in,max}}$ is the maximum allowed concentration of contaminant c at the inlet of unit u .

Maximum Outlet Concentration at the Water-Using Units.

$$\sum_w (\text{CW}_{w,c} \text{FWU}_{w,u}) + \sum_{u^*} \text{ZUU}_{u^*,u,c} + \sum_r \text{ZRU}_{r,u,c} + \Delta M_{u,c} \leq C_{u,c}^{\text{out,max}} (\sum_{u^*} \text{FUU}_{u,u^*} + \sum_r \text{FUR}_{u,r} + \sum_{u^*} \text{FUU}_{u,u^*} + \sum_s \text{FUS}_{u,s}) \quad \forall u, c \quad (5)$$

where $C_{u,c}^{\text{out,max}}$ is the maximum allowed concentration of contaminant c at the outlet of unit u .

Contaminant Balance at the Regeneration Processes.

$$\text{ZR}_{r,c}^{\text{in}} = \sum_w (\text{CW}_{w,c} \text{FWR}_{w,r}) + \sum_u \text{ZUR}_{u,r,c} + \sum_{r^*} \text{ZRR}_{r^*,r,c} \quad \forall r, c \quad (6)$$

$$\text{ZR}_{r,c}^{\text{out}} = \sum_u \text{ZRU}_{r,u,c} + \sum_{r^*} \text{ZRR}_{r,r^*,c} + \sum_s \text{ZRS}_{r,s,c} \quad \forall r, c \quad (7)$$

where $\text{ZR}_{r,c}^{\text{in}}$ is the mass flow of contaminant c going into regeneration process r and $\text{ZR}_{r,c}^{\text{out}}$ is the mass flow of contaminant c leaving regeneration process r . If the regeneration process is defined by fixed outlet concentration, eq 8 is used.

$$\text{ZR}_{r,c}^{\text{out}} = \text{ZR}_{r,c}^{\text{in}} (1 - \text{XCR}_{r,c}) + (\sum_w \text{FWR}_{w,r} + \sum_u \text{FUR}_{u,r} + \sum_{r^*} \text{FRR}_{r^*,r}) \text{CRF}_{r,c}^{\text{out}} \text{XCR}_{r,c} \quad \forall r, c \quad (8)$$

where $\text{CRF}_{r,c}^{\text{out}}$ is the outlet concentration of contaminant c in regeneration process r and $\text{XCR}_{r,c}$ is a binary parameter that indicates if contaminant c is treated by regeneration process r . We

assume that $CRF_{r,c}^{out}$, the concentration of the treated contaminant is known and constant.

For the cases in which the regeneration process is assumed to have fixed rate of removal, eq 9 is used.

$$ZR_{r,c}^{out} = ZR_{r,c}^{in} (1 - RR_{r,c}) \quad \forall r, c \quad (9)$$

where $RR_{r,c}$ is a given rate of removal of contaminant c in regeneration process r .

Capacity of the Regeneration Processes.

$$CAP_r = \sum_w FWR_{w,r} + \sum_u FUR_{u,r} + \sum_{r^*} FRR_{r^*,r} \quad \forall r \quad (10)$$

where CAP_r is capacity of regeneration process r .

Maximum Allowed Discharge Concentration.

$$\sum_u ZUS_{u,s,c} + \sum_r ZRS_{r,s,c} \leq C_{s,c}^{discharge, max} \left(\sum_u FUS_{u,s} + \sum_r FRS_{r,s} \right) \quad \forall s, c \quad (11)$$

where $C_{s,c}^{discharge, max}$ is the maximum allowed concentration at sink s .

Minimum Flow Rates. It is well-known that many solutions of the water problem may include small flow rates that are impractical. To avoid these we use the following constraints:

$$FWU_{w,u} \geq FWU_{w,u}^{min} YWU_{w,u} \quad \forall w, u \quad (12)$$

$$FUU_{u,u^*} \geq FUU_{u,u^*}^{min} YUU_{u,u^*} \quad \forall u, u^* \quad (13)$$

$$FUS_{u,s} \geq FUS_{u,s}^{min} YUS_{u,s} \quad \forall u, s \quad (14)$$

$$FUR_{u,r} \geq FUR_{u,r}^{min} YUR_{u,r} \quad \forall u, r \quad (15)$$

$$FRU_{r,u} \geq FRU_{r,u}^{min} YRU_{r,u} \quad \forall r, u \quad (16)$$

$$FRR_{r,r^*} \geq FRR_{r,r^*}^{min} YRR_{r,r^*} \quad \forall r, r^* \quad (17)$$

$$FRS_{r,s} \geq FRS_{r,s}^{min} YRS_{r,s} \quad \forall r, s \quad (18)$$

These constraints use a set of binary variables ($YWU_{w,u}$, YUU_{u,u^*} , $YUS_{u,s}$, $YUR_{u,r}$, $YRU_{r,u}$, YRR_{r,r^*} , and $YRS_{r,s}$) that are equal to one when the corresponding flow rate is different from zero and zero otherwise.

Maximum Flow Rates. To ensure that the connections do not surpass maximum values, we use the following constraints:

$$FWU_{w,u} \leq FWU_{w,u}^{max} YWU_{w,u} \quad \forall w, u \quad (19)$$

$$FUU_{u,u^*} \leq FUU_{u,u^*}^{max} YUU_{u,u^*} \quad \forall u, u^* \quad (20)$$

$$FUS_{u,s} \leq FUS_{u,s}^{max} YUS_{u,s} \quad \forall u, s \quad (21)$$

$$FUR_{u,r} \leq FUR_{u,r}^{max} YUR_{u,r} \quad \forall u, r \quad (22)$$

$$FRU_{r,u} \leq FRU_{r,u}^{max} YRU_{r,u} \quad \forall r, u \quad (23)$$

$$FRR_{r,r^*} \leq FRR_{r,r^*}^{max} YRR_{r,r^*} \quad \forall r, r^* \quad (24)$$

$$FRS_{r,s} \leq FRS_{r,s}^{max} YRS_{r,s} \quad \forall r, s \quad (25)$$

The values of the maximum flow rates $FWU_{w,u}^{Max}$ and $FUS_{u,s}^{Max}$ are lower or equal to maximum flow rate imposed through unit u , that is $FWU_{w,u}^{Max} \leq FU_u^{max}$ and $FUS_{u,s}^{Max} \leq FU_u^{max}$ and $FRS_{r,s}^{Max}$ is lower than or equal to the maximum flow rate imposed through regeneration unit r , $FRS_{r,s}^{Max} \leq FR_r^{max}$. The rest of the maximum flow rates are limited by the maximum flow rate imposed through the units they connect, that is: $FUU_{u,u^*}^{Max} \leq \min\{FU_u^{max}, FU_{u^*}^{max}\}$, $FUR_{u,r}^{Max} \leq \min\{FU_u^{max}, FR_r^{max}\}$, $FRU_{r,u}^{Max} \leq \min\{FR_r^{max}, FU_u^{max}\}$, $FRR_{r,r^*}^{Max} \leq \min\{FR_r^{max}, FR_{r^*}^{max}\}$.

The contaminant mass flow rates are enough and no new variables are needed in the case of mixing nodes. However, the splitting nodes at the outlet of each unit and the regeneration units need constraints that will reflect that all these contaminant flows and the total mass flows are consistent with the concentrations of the different contaminants. Thus we add the corresponding relations.

Contaminant Mass Flow Rates.

$$ZUU_{u,u^*,c} = FUU_{u,u^*} C_{u,c}^{out} \quad \forall u, u^*, c \quad (26)$$

$$ZUS_{u,s,c} = FUS_{u,s} C_{u,c}^{out} \quad \forall u, s, c \quad (27)$$

$$ZUR_{u,r,c} = FUR_{u,r} C_{u,c}^{out} \quad \forall u, r, c \quad (28)$$

$$ZRU_{r,u,c} = FRU_{r,u} CR_{r,c}^{out} (1 - XCR_{r,c}) + FRU_{r,u} CRF_{r,c}^{out} XCR_{r,c} \quad \forall r, u, c \quad (29)$$

$$ZRR_{r,r^*,c} = FRR_{r,r^*} CR_{r,c}^{out} (1 - XCR_{r,c}) + FRR_{r,r^*} CRF_{r,c}^{out} XCR_{r,c} \quad \forall r, r^*, c \quad (30)$$

$$ZRS_{r,s,c} = FRS_{r,s} CR_{r,c}^{out} (1 - XCR_{r,c}) + FRS_{r,s} CRF_{r,c}^{out} XCR_{r,c} \quad \forall r, s, c \quad (31)$$

where $C_{u,c}^{out}$ is the outlet concentration of contaminant c in unit u , and $CR_{r,c}^{out}$ is the outlet concentration of the not treated contaminant c in regeneration r (which is a variable), $CRF_{r,c}^{out}$ is the outlet concentration of the treated contaminant c in regeneration r (which is a parameter), and $XCR_{r,c}$ is a binary parameter that defines c is treated by regeneration r . Finally, we write

$$CR_{r,c}^{out, min} \leq CR_{r,c}^{out} \leq CR_{r,c}^{out, max} \quad \forall r, c \quad (32)$$

$$C_{u,c}^{out, min} \leq C_{u,c}^{out} \leq C_{u,c}^{out, max} \quad \forall u, c \quad (33)$$

We most certainly need eq 33, but eq 32 may be optional. In addition to the bound contraction arithmetic used to define minimum and maximum flow rates between two units/processes, bound arithmetic on the outlet concentrations is

also used. Those are

$$C_{u,c}^{\text{out},\min} = \max \left\{ C_{u,c}^{\text{out},\min}, \left(\min \left\{ \begin{array}{l} \text{Min}_{u^*} \{ C_{u^*,c}^{\text{out},\min} \} \\ \text{Min}_w \{ CW_{w,c} \} \\ \text{Min}_{r^* \forall XCR_{r^*,c}=1} \{ CRF_{r^*,c}^{\text{out}} \} \end{array} \right\} \prod_r (1 - RR_{r,c}) \right) + \frac{\Delta M_{u,c}}{FU_u^{\max}} \right\} \quad \forall u, c \quad (34)$$

$$C_{u,c}^{\text{out},\max} = \min \left\{ C_{u,c}^{\text{out},\max}, \left(\min \left\{ C_{u^*,c}^{\text{in},\max}, \max \left\{ \begin{array}{l} \text{Max}_{u^*} \{ C_{u^*,c}^{\text{out},\max} \} \\ \text{Max}_w \{ CW_{w,c} \} \\ \text{Max}_{r^* \forall XCR_{r^*,c}=1} \{ CRF_{r^*,c}^{\text{out}} \} \\ \text{Max}_{r^* \forall XCR_{r^*,c}=0} \{ CR_{r^*,c}^{\text{out}} (1 - RR_{r^*,c}) \} \end{array} \right\} \right) + \frac{\Delta M_{u,c}}{FU_u^{\min}} \right\} \quad \forall u, c \quad (35)$$

$$CR_{r,c}^{\text{out},\min} = \max \left\{ CR_{r,c}^{\text{out},\min}, \left(\min \left\{ \begin{array}{l} \text{Min}_u \{ C_{u,c}^{\text{out},\min} \} \\ \text{Min}_w \{ CW_{w,c} \} \\ \text{Min}_{r^* \forall XCR_{r^*,c}=1} \{ CRF_{r^*,c}^{\text{out}} \} \end{array} \right\} \prod_{r^*} (1 - RR_{r^*,c}) \right) (1 - RR_{r,c}) \right\} \quad \forall r, c \quad (36)$$

$$CR_{r,c}^{\text{out},\max} = \min \left\{ CR_{r,c}^{\text{out},\max}, \left(\min \left\{ C_{u,c}^{\text{in},\max}, \max \left\{ \begin{array}{l} \text{Max}_u \{ C_{u,c}^{\text{out},\max} \} \\ \text{Min}_w \{ CW_{w,c} \} \\ \text{Max}_{r^* \forall XCR_{r^*,c}=1} \{ CRF_{r^*,c}^{\text{out}} \} \\ \text{Max}_{r^* \forall XCR_{r^*,c}=0} \{ CR_{r^*,c}^{\text{out}} (1 - RR_{r^*,c}) \} \end{array} \right\} \right) (1 - RR_{r,c}) \right\} \quad \forall r, c \quad (37)$$

Equation 34 defines the minimum outlet concentrations for the units as the maximum value between the current minimum outlet concentration and the minimum value that can be reached through bound arithmetic of the eqs 1 and 3. Following the same idea, eq 35 is defined for the maximum outlet concentrations of water-using units. Equations 36 and 37 are related to the regeneration processes and the bounds arithmetic is defined by eqs 2 and 6–9.

Objective Functions. To overcome the nonconvexities created by bilinear terms, we present examples that minimize freshwater consumption given by

$$\min FW = \sum_w \left(\sum_u FWU_{w,u} + \sum_r FWR_{w,r} \right) \quad (38)$$

Additionally, we show examples that minimize total annual cost. These cases have also nonlinearity on the concave terms (capital cost) in the objective function. The total annual cost (TAC) is

given by

$$\max TAC = OP \left(\sum_w \alpha_w \left(\sum_u FWU_{w,u} + \sum_r FWR_{w,r} \right) + \sum_r OPN_r FR_r \right) - af FCI \quad (39)$$

where OPN_r are the operational cost of the regeneration processes and OP is the hours of operation per year. The last term is the annualized capital cost, where af is any factor that annualizes the capital cost (usually $1/N$, where N is the number of years of depreciation) and CCR_r is the capital cost coefficient of the regeneration processes. Finally, all the variables must be non-negative.

$$FCI = \sum_w \left(\begin{array}{l} \sum_u (FWUC_{w,u} YWU_{w,u} + VWUC_{w,u} FWU_{w,u}) \\ + \sum_r (FWRC_{w,r} YWR_{w,r} + VWRC_{w,r} FWR_{w,r}) \\ + \sum_s (FWSC_{w,s} YWS_{w,s} + VWSC_{w,s} FWS_{w,s}) \end{array} \right) + \sum_u \left(\begin{array}{l} \sum_{u^*} (FUUC_{u,u^*} YUU_{u,u^*} + VUUC_{u,u^*} FUU_{u,u^*}) \\ + \sum_r (FURC_{u,r} YUR_{u,r} + VURC_{u,r} FUR_{u,r}) \\ + \sum_s (FUSC_{u,s} YUS_{u,s} + VUSC_{u,s} FUS_{u,s}) \end{array} \right) + \sum_r \left(\begin{array}{l} FRC_r YR_r + VRC_r (FR_r)^{0.7} \\ + \sum_u (FRUC_{r,u} YRU_{r,u} + VRUC_{r,u} FRU_{r,u}) \\ + \sum_{r^*} (FRRC_{r,r^*} YRR_{r,r^*} + VRRC_{r,r^*} FRR_{r,r^*}) \\ + \sum_s (FRSC_{r,s} YRS_{r,s} + VRSC_{r,s} FRS_{r,s}) \end{array} \right) \quad (40)$$

One of the decisions that have to be made is regarding the variable of that bilinear term that is being partitioned. For water management problems, the bilinear terms generated by the splitters are formed by the following variables: Outlet concentration of the processes (water-using units and regeneration processes); and, flow rates. Thus, one must choose to partition outlet concentrations of processes, flow rates or both. The choice has effect on the tightness of the lower bound, the increase in number of binaries due to partitions/linearizations and the efficiency of the MILP formulation. Following Faria and Bagajewicz,¹ we show the number of variables that need to be partitioned in each case, comparing partitioning of flow rates and partitioning of concentrations (Table 1). Note that the number of flow rate variables is usually higher than the number of outlet concentrations variables (only the highlighted ones are not). Faria and Bagajewicz¹ discussed in detail the merits of each choice.

4. WATER MANAGEMENT RESULTS

We show now several examples that illustrate the effectiveness of the method. Examples 1–4 are multicomponent refinery examples; the first and the second without regeneration processes and the third with regeneration units, all three solving for minimum freshwater. All these four examples do not require any elimination procedure because they find the solution at the first LB. Example 5 is added to compare our method's performance with that of Karupiah and Grossmann.² In this case, the elimination procedure requires more than one iteration, so we use it to illustrate the performance of different options. Examples 6 and 7 are added to illustrate the performance of the method

Table 1. Comparison of Number of Partitioned Variables

number of units	flows	C^{out} (number of contaminants)									
		1	2	3	4	5	6	7	8	9	10
2	4	2	4	6	8	10	12	14	16	18	20
3	9	3	6	9	12	15	18	21	24	27	30
4	16	4	8	12	16	20	24	28	32	36	40
5	25	5	10	15	20	25	30	35	40	45	50
6	36	6	12	18	24	30	36	42	48	54	60
7	49	7	14	21	28	35	42	49	56	63	70
8	64	8	16	24	32	40	48	56	64	72	80
9	81	9	18	27	36	45	54	63	72	81	90
10	100	10	20	30	40	50	60	70	80	90	100
11	121	11	22	33	44	55	66	77	88	99	110
12	144	12	24	36	48	60	72	84	96	108	120
13	169	13	26	39	52	65	78	91	104	117	130
14	196	14	28	42	56	70	84	98	112	126	140
15	225	15	30	45	60	75	90	105	120	135	150
16	256	16	32	48	64	80	96	112	128	144	160
17	289	17	34	51	68	85	102	119	136	153	170
18	324	18	36	54	72	90	108	126	144	162	180
19	361	19	38	57	76	95	114	133	152	171	190
20	400	20	40	60	80	100	120	140	160	180	200

when cost is minimized. We also use a problem from Karuppiah and Grossmann² to compare. Example 8, illustrates that one can find solutions applying different discretization intervals to key variables. Example 9 is added to show that the method can solve total water systems²¹ minimizing cost. Finally, example 10 is one that presents computational challenges: variable costs in addition to fixed costs of connections, water using units with variable flow rates (some problems assume fixed flow rate) and regeneration processes competing for contaminants to treat. In this case, our solution procedure is less efficient than BARON, although it finds the answer at the root node.

4.1. Example 1: A Refinery Example. This example is the classical small refinery example presented by Wang and Smith.²² The objective is to minimize the freshwater consumption of a water system with three water-using units, three contaminants and one regeneration process. The limiting data of the water-using units used in this example is presented in Table 2. Note that these water-using units do not have fixed flow rate predefined by the problem.

The available freshwater source is free of contaminants, and the available regeneration process is a foul water stripper with a rate of removal of 0.999 for H₂S.

Wang and Smith²² used a graphical approach to obtain the solution of this problem (55.5 t/h). We partition concentrations and used several different numbers of intervals, from 1 interval, to many more. In addition we used both types of partitioning methods: *Direct discretization* and *McCormick's envelopes*. We also tried the three different linearization procedures to linearize the product of continuous and binary variables of both lower bound models. Finally, we run it for partitioned concentrations as well as for partitioned flow rates. All of these alternatives find the global optimum solution (55.47 t/h) at the root node.

In the case of 1 interval and direct partitioning of flow rates using procedure 2 (DPP2) the model has 32 binary variables and

Table 2. Limiting Data of Example 2

process	contaminant	mass load (kg/h)	$C^{\text{in,max}}$	$C^{\text{out,max}}$
			(ppm)	(ppm)
1	distillation	HC	0.675	0
		H ₂ S	18	0
		salts	1.575	0
2	HDS	HC	3.4	20
		H ₂ S	414.8	300
		salts	4.59	45
3	desalter	HC	5.6	120
		H ₂ S	1.4	20
		salts	520.8	200

264 continuous variables. Conversely, in the case of 1 interval and direct partitioning of concentration using DPP2, the model has 13 binary variables and 145 original continuous variables. Because there are no lower and upper bounds for the flows in this problem, we do not include in the above counts the unneeded binaries corresponding to equations (12–25). The number of continuous variables is increased from the original value to a larger one because of the linearization procedure, which is different depending of which one is used.

Applying the suggested methodology using one interval, the optimum solution (55.47 t/h) is found in 0.10 and 0.16 s, for discretized concentrations and discretized flow rates using DPP2, respectively. As stated above, in all these examples we only report the running time, not including the model preprocessing/generation time, which is about 1.6 s and the solution reporting time, which is about 0.7 s (slightly larger for larger problems). The solution is actually obtained at the root node as the lower bound renders an objective function equal to the global minimum. In other words, there is no need for an interval elimination procedure. Although the solution value found is nearly the same (ours is slightly lower), the network is different. Figure 1 compares both.

4.2. Example 2: Multicontaminant Water System without Regeneration—Freshwater Minimization. This example is the refinery case presented by Koppol et al.¹¹ This example has four key contaminants (salts, H₂S, organics, and ammonia) and six water-using units. The limiting data of the water-using units are shown in Table 3. This network without reuse consumes 144.8 t/h of freshwater and the objective is to minimize freshwater consumption. The flow rate through the water-using units are not predefined and they can vary from the limiting low flow rate to a maximum allowed flow rate. The minimum freshwater consumption found by Koppol et al.¹¹ is 119.33 t/h, which was not originally solved to guaranteed global optimality.

In this problem, we tried the same options of number of intervals, discretization methods and discretized variables as in example 2. A global optimum solution (119.33 t/h) is found in 0.14 s. The lower bound gives the optimum solution and thus it is found at the root node when *McCormick's envelopes* and when *Direct partitioning* of concentrations are used. A LB that is different from the optimum solution is obtained when *Direct partitioning* of flow rates are applied for less than 10 intervals. The minimum freshwater consumption is the same as that of Koppol et al.,¹¹ but the network obtained is different, which indicates that this problem is degenerate. Both networks are presented in Figure 2. The same comments regarding the time reported as in example 2 hold.

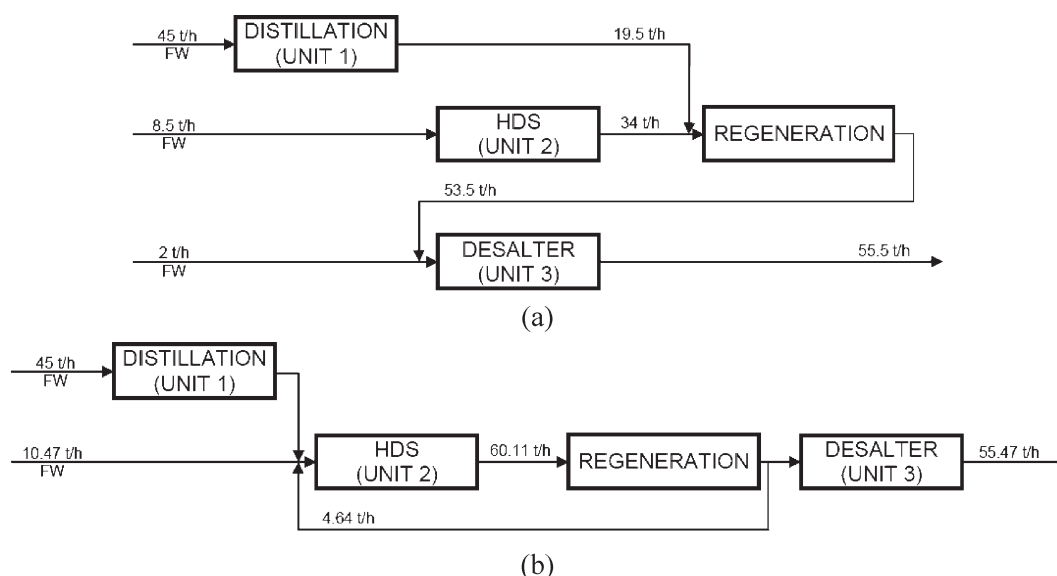


Figure 1. Optimum network of example 1. (a) Wang and Smith's ²² solution and (b) our solution.

Table 3. Limiting Data of Example 2

process	contaminant	mass load (kg/h)	$C_{in,max}$ (ppm)	$C_{out,max}$ (ppm)
1 caustic treating	salts	0.18	300	500
	organics	1.2	50	500
	H ₂ S	0.75	5000	11000
	ammonia	0.1	1500	3000
2 distillation	salts	3.61	10	200
	organics	100	1	4000
	H ₂ S	0.25	0	500
	ammonia	0.8	0	1000
3 amine sweetening	salts	0.6	10	1000
	organics	30	1	3500
	H ₂ S	1.5	0	2000
	ammonia	1	0	3500
4 merox-I sweetening	salts	2	100	400
	organics	60	200	6000
	H ₂ S	0.8	50	2000
	ammonia	1	1000	3500
5 hydrotreating	salts	3.8	85	350
	organics	45	200	1800
	H ₂ S	1.1	300	6500
	ammonia	2	200	1000
6 desalting	salts	120	1000	9500
	organics	480	1000	6500
	H ₂ S	1.5	150	450
	ammonia	0	200	400

4.3. Example 3: Multicontaminant Water System with Regeneration—Freshwater Minimization. In this example the network presented in example 3 is solved with the addition of potential regeneration processes that are modeled as processes with fixed outlet concentrations. Three regeneration processes are available: Reverse osmosis, which reduces salts to 20 ppm; API separator followed by ACA, which reduces organics to 50 ppm; and, Chevron wastewater treatment, which reduces H₂S to 5 ppm and ammonia to 30 ppm. The optimum solution obtained by Koppol et al.¹¹ reaches a minimum freshwater consumption of 33.571 t/h. As in the previous case, they did not solve guaranteeing global optimality.

In this problem, we also tried the same options of number of intervals, discretization methods and discretized variables as in the previous examples. In all cases where we partitioned con-

centrations or partitioned flow rates using *McCormick's envelopes*, we obtained the same result: a lower bound solution of 33.571 t/h at the root node with only one interval. This solution corresponds to the global optimum solution of this problem. The best solution (fastest one) is found in approximately 0.56 s using MCP2 with discrete concentrations. The minimum freshwater consumption is the same as that of Koppol et al.¹¹

Although the minimum freshwater consumption is obtained, the found network presents very small flow rates such as 0.06 t/h. To avoid these small flow rates we added a minimum allowed flow rates of 1 t/h for the connections (eqs 12–18). In this case, a lower bound equal to the global solution is also found at the root node, but the original model (upper bound model) does not find a feasible solution at the root node. Thus, the method has to keep looking for a solution and eliminating parts of the feasible region until the upper bound model finds the global optimum solution. We find the solution in 75.71 s (1 min 15.71 s) using the standard elimination procedure with *active upper bounding* discretizing concentrations (2 intervals) through MCP2.

The networks obtained by Koppol et al.¹¹ and ours are presented in Figure 3. The same comments regarding the time reported as in example 3 hold.

When flow rates are partitioned using *Direct partitioning*, the lower bound is no longer equal to the global optimum solution and interval elimination is needed. In fact, the lower bound generated by this option is equal to zero. As discussed by Faria and Bagajewicz,¹ the lower bound can be further improved when a preprocessing step includes forbidden connections that cannot exist. In the WAP, the following rule was proposed:

$$FUU_{u*,u}^{\max} = 0 \text{ if } C_{u,c}^{\text{in},\max} < \bar{C}_c^{\min} \quad (41)$$

$$FRU_{r,u}^{\max} = 0 \text{ if } C_{u,c}^{\text{in},\max} < \bar{C}_c^{\min} \quad (42)$$

where \bar{C}_c^{\min} is the minimum concentration of contaminant c in the system, which is defined by

$$\bar{C}_c^{\min} = \min\{\text{Min}_u\{C_{u,c}^{\text{out},\min}\}, \text{Min}_r\{CR_{r,c}^{\text{out},\min}\}, \text{Min}_w\{CW_{w,c}\}\} \quad (43)$$

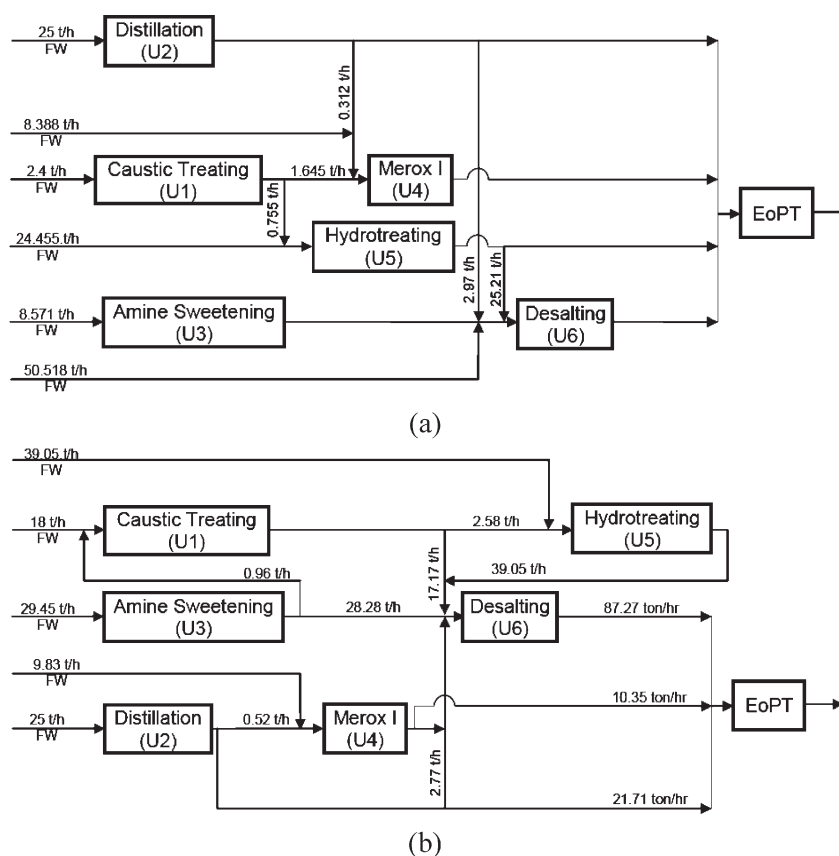


Figure 2. Optimum network of example 2. (a) Koppol et al.¹¹ and (b) this article.

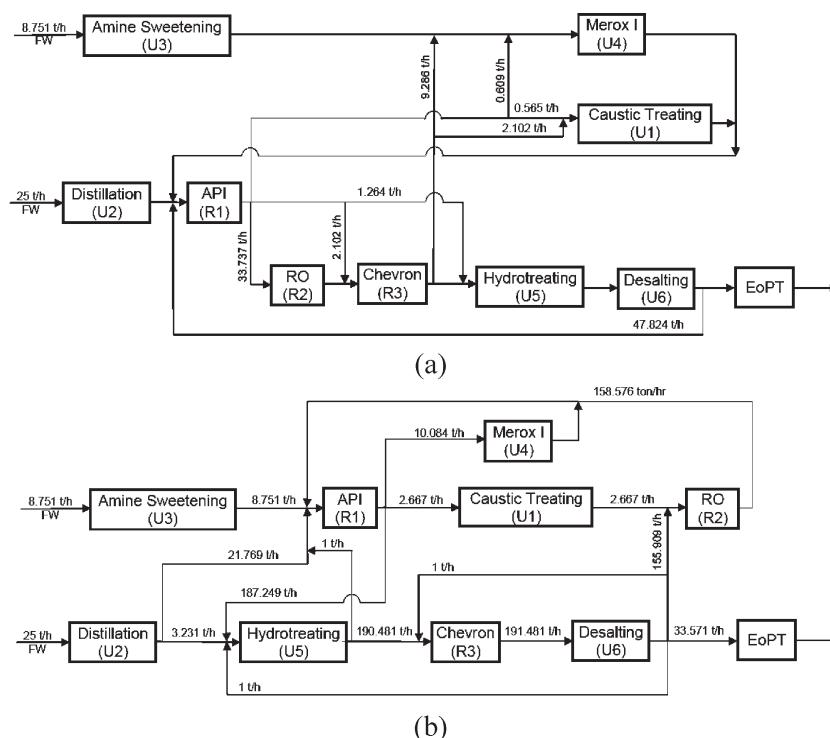


Figure 3. Optimum network of example 3. (a) Koppol et al.¹¹ and (b) ours.

Now, adding the forbidden connections, the *Direct partitioning* of flow rates is tighter but still not as tight as using the *McCormick's envelopes*.

Without a required minimum flow rates through the connections these lower bounds keep constant (16.1185 t/h) for up to 10 intervals.

Table 4. Water Using Units Limiting Data of Example 4

process	contaminant	mass load (kg/h)	$C^{\text{in,max}}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	

Table 5. Regeneration Processes Data of Example 4

process	contaminant	removal ratio (%)
1	A	95
	B	0
2	A	0
	B	95

4.4. Example 4: Multicontaminant Water System with Regeneration—Freshwater + Regeneration Flow Rate Minimization. This example was proposed by Karuppiyah and Grossmann.² It is a network involving two water using units, two treatment processes and two contaminants. Unlike the previous examples, in this case the water-using units have fixed flow rates, the treatment processes are modeled having a fixed efficiency and the objective is to minimize the summation of freshwater flow rate and the flow rate treated by the regeneration processes. The rationale for such an objective, according to the authors, is that the integrated system is being solved and a network with minimum freshwater consumption would have a higher combined freshwater and treated flow rate. There is a maximum discharge of the effluents to the sink (10 ppm for both contaminants A and B). Tables 4 and 5 show the data of this example.

The global optimal solution (117.05 t/h) is found by Karuppiyah and Grossmann² in 37.72 s. In our case, the solution is not always found at the root node. We report the times even though they correspond to different processors.

Table 6 presents the solution of this problem using the different lower bound models when outlet concentrations are partitioned. These solutions are the ones that give the lowest computational time.

The solution partitioning flow rates in 2 intervals and using McCormick's envelopes took 11,795 s and 35 iterations when the standard procedure was used. We also looked into using branch and bound after bound contraction through interval elimination cannot progress further. Details of this are given by Faria and Bagajewicz.¹ Finally, Table 7 provides details and Figure 4 shows the optimum network.

4.5. Example 5: Multicontaminant Water System with Regeneration—Cost Minimization. This example is a two contaminant, three water-using unit, and three regeneration processes problem proposed and solved by Karuppiyah and Grossmann.² This problem minimizes total annual cost and assumes fixed flow rates through the water-using units and regeneration processes with fixed rate of removal. Maximum concentration at the disposal is 10 ppm for both contaminants. The data used for example 6 is presented in Tables 8 and 9. The cost of freshwater is \$1/t, the annualized factor is 0.1 and the plant runs 8000 h/year. The authors found the global optimal solution (\$381,751.35/year) in 13.21 s. Later, Bergamini et al.⁷ solved this problem to proven global optimality in 3.75 s.

We partitioned concentrations in the water using units and flow rates through the regeneration processes (because of the concave objective function) and used 4 intervals, resulting in a model (MCP2) that has 52 binary variables and 585 continuous

variables. With the presented method pre-excluding the infeasible connections, we find the optimal solution in 0.41 s at the root node. This lower bound model generates an objective function of \$378,215.14 per year, which is 0.93% lower than the objective function and thus complies with the required tolerance. If forbidding of infeasible connections is not used, the same lower bound model (MCP2 with partitioned concentrations and 4 intervals) generates a value of \$168,140.03 per year. The global solution is the same as that of Karuppiyah and Grossmann² and Bergamini et al.⁷ The obtained network is presented in Figure 5.

4.6. Example 6: Multicontaminant System with Regeneration—Cost Minimization. This example is also taken from Karuppiyah and Grossman.² It involves two contaminants and has four water-using units and two regeneration processes. Data related to the water-using units and regeneration processes are presented in Tables 10 and 11. The same economic data and discharge limits (10 ppm) are applied for this problem.

We partitioned concentrations and flow rates through the regeneration processes as in example 6 and used two intervals. All the models (DDP2, DDP3, MCP2, and MCP3) that discretize concentrations in two intervals have a lower bound objective function of \$871,572.22 (which is 0.28% lower than the global solution) and thus find the optimal solution (\$874,057.37/year) in approximately 0.25 s at the root node. The resulting model has 24 binary variables and 408 continuous variables (DDP2 and MCP2) or 254 continuous variables (DDP3 and MCP3). The solution is presented in Figure 6.

4.7. Example 7: Multicontaminant Water System with Regeneration—Cost Minimization. This example is a large system presented by Karuppiyah and Grossmann.² It involves three contaminants and has five water-using units with fixed flow rates and three regeneration processes. The data for this example is presented in Tables 12 and 13. Additionally, the discharge limit of all the contaminants is 10 ppm.

For this example, we partition concentrations and apply the interval elimination procedure only on the outlet concentrations and flow rates through the regeneration processes. Note that even without applying the reduction procedure in the flow rates through the connection of their bounds may be influenced by the contraction of the regenerated flow rate's bounds because of the bounds arithmetic.

Instead of using the standard procedure, we use the *one-pass, extended interval forbidding, exhaustive elimination with active upper bounding*.

Karuppiyah and Grossmann² found the minimum TAC (global solution) of this of \$1,033,810.95/year. We found the same network in 30.15 s in the first iteration using the McCormick's envelopes model with partitioned concentrations and flow rates through the regeneration processes (because of the concave function). This lower bound model with 2 intervals has 48 binary variables and 919 continuous variables. This network also has a small flow rate (0.04 t/h). Thus, we solve the problem using the MINLP formulation, which requires a minimum flow rate of 1 t/h through the connection. With this new constraint the found minimum TAC is \$1,033,859.85 in 73.79s after the first iteration. The network corresponding to this solution is presented in Figure 7. The network contains many recycles, which form the practical point of view could be rejected as too complex.

4.8. Example 8: Single-Contaminant Water System with Regeneration—Cost Minimization. Example 8 is a single contaminant water system presented by Faria and Bagajewicz,²¹ which has 4 water-using units and 3 regeneration processes (2 water pretreatments and 1 end-of-pipe treatment). Table 14 shows the limiting data of the water-using units.

Table 6. Summary of Results for Discrete Concentration of Example 5

LB model	discretized variable	first LB	initial no. of intervals	linearization procedure	iterations	time
direct partitioning	concentrations	116.31 t/h	10	P2	0	1.59 s
McCormick envelopes	concentrations	116.31 t/h	10	P2	0	1.57 s

Table 7. Summary of Results for Partitioned Flow Rates of Example 5

branching variable	investigated subproblems	linearization procedure	time
outlet concentrations	4	MCP2	23.73 s
flow rates	4	MCP2	40.93 s

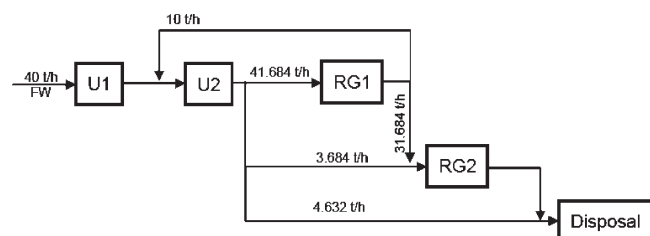


Figure 4. Optimum network of example 4.

Table 8. Water Using Units Limiting Data of Example 5

process	contaminant	mass load (kg/h)	$C^{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	
3	A	1	50	60
	B	1	50	

Table 9. Regeneration Processes Data of Example 5

process	contaminant	removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16800
	B	0		
2	A	80	0.003	24000
	B	90		
3	A	0	0.0067	12600
	B	95		

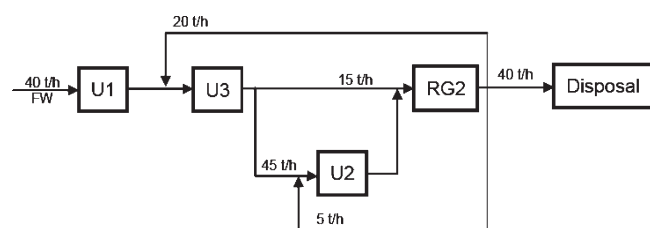


Figure 5. Optimum network of example 5.

One external freshwater source is assumed, but the two water treatment units are able to provide two different qualities of freshwater. Pretreatment 1 can bring the freshwater down to 10 ppm and pretreatment 2 can further treat it down to 0 ppm. Pretreatment 1 has

Table 10. Water Using Units Limiting Data of Example 6

process	contaminant	mass load (kg/h)	$C^{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
2	A	1	50	50
	B	1	50	
3	A	1	50	60
	B	1	50	
4	A	2	50	70
	B	2	50	

Table 11. Regeneration Processes Data of Example 6

process	contaminant	removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16800
	B	0		
2	A	0	0.0067	12600
	B	90		

an operating cost of \$0.30/t and a capital cost of \$8,500/t^{0.7} with a maximum inlet concentration of 500 ppm. The operating cost of pretreatment 2 is \$0.50/t, and the capital cost is \$10,500/t^{0.7}, and maximum inlet concentration is 20 ppm. The end-of-pipe treatment has an outlet concentration of 25 ppm, which coincides with the discharge limit. The operating cost of the end of pipe treatment is OPN_r (\$/t) = 10067, and the investment cost is CCR_r (\$/t^{0.7}) = 19,400. The capital costs with connections are presented in Table 15. Freshwater is assumed to be α_f (\$/t) = 0.3 and the system operates 8600 h per year.

The optimum solution is the same presented by Faria and Bagajewicz,²¹ and it was found in 3 CPUs to guaranteed global optimality. The corresponding network, which has a TAC of \$410,277, is presented in Figure 8.

4.9. Example 9: Multicontaminant Water System with Regeneration—Cost Minimization. This problem was presented by Kuo and Smith,²³ which was solved using graphical approach for the design of effluent system and the cost evaluation considered freshwater cost and regeneration costs. Later, Gunaratnam et al.¹² and Alva-Argaez et al.¹⁴ introduced piping costs and solved the problem using mathematical programming and minimizing the total annual cost considering freshwater cost, operating cost of regeneration processes and capital cost of regeneration processes and piping. The data for the processes and the regeneration units is shown in Tables 16 and 17. The discharge limits of this system are 20 ppm for HC, 5 ppm for H₂S, and 100 ppm for SS. The freshwater cost is \$0.2/t and the system operates 8600 h per year. A 10% rate of discount is assumed. Table 18 shows the distances among processes.

Thus, the piping costs assuming a velocity of 1 m/s are given by

$$FIJC_{i,j} = 124.6d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \quad (44)$$

$$VIJC_{i,j} = 1.001d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \quad (45)$$

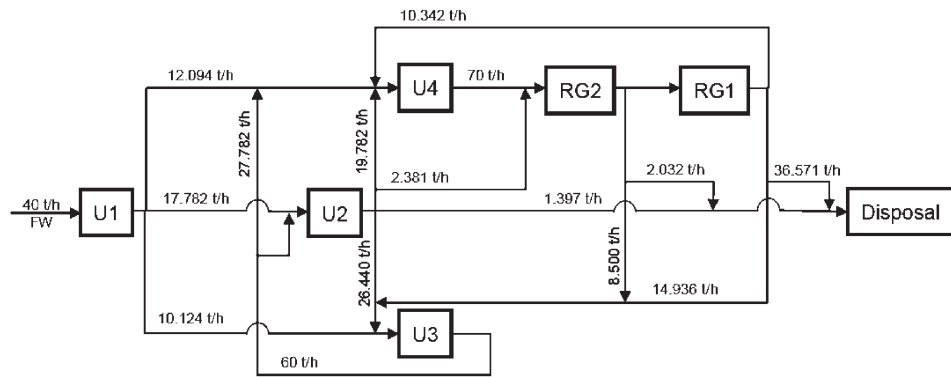


Figure 6. Optimum network of example 6.

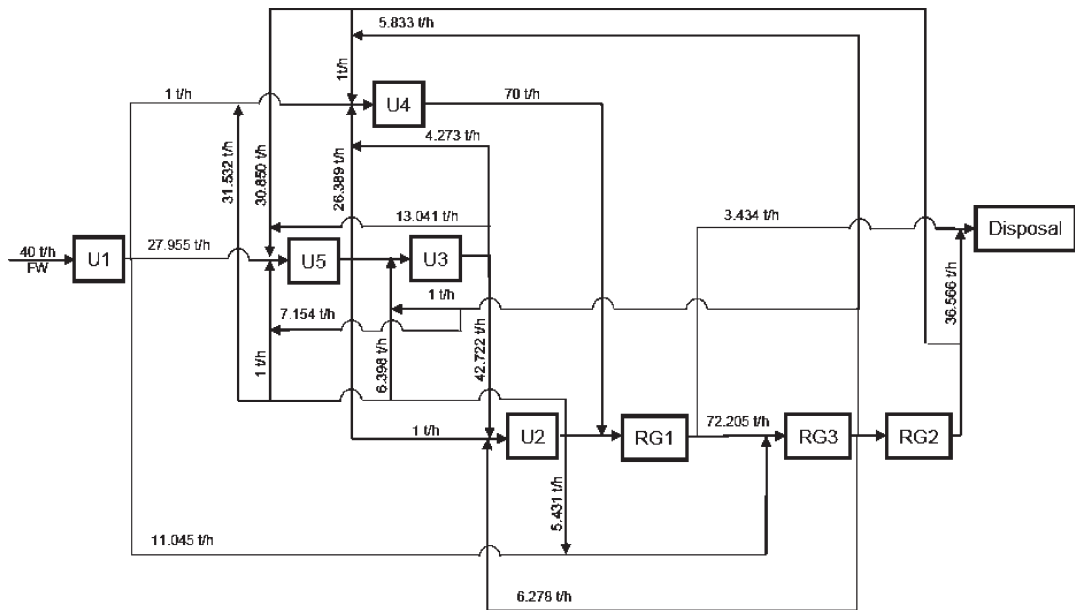


Figure 7. Optimum network of example 7.

Table 12. Water Using Units Limiting Data of Example 7

process	contaminant	mass load (kg/h)	$C_{in,max}$ (ppm)	F (t/h)
1	A	1	0	40
	B	1.5	0	
	C	1	0	
2	A	1	50	50
	B	1	50	
	C	1	50	
3	A	1	50	60
	B	1	50	
	C	1	50	
4	A	2	50	70
	B	2	50	
	C	2	50	
5	A	1	25	80
	B	1	25	
	C	0	25	

Table 13. Regeneration Processes Data of Example 7

process	contaminant	removal ratio (%)	OPN_r	VRC_r
1	A	95	1	16800
	B	0		
	C	0		
2	A	0	0.04	9500
	B	0		
	C	95		
3	A	0	0.0067	12600
	B	95		
	C	0		

Table 14. Limiting Data for Example 8

process number	mass load of contaminant	C_{in} (ppm)	C_{out} (ppm)
1	2 kg/h	0	100
2	5 kg/h	20	100
3	30 kg/h	50	800
4	4 kg/h	400	800

The best known solution¹⁴ for this problem minimizing TAC is \$616,824. We include this problem because it presents several

Table 15. Capital Costs of the Connections

	unit 1	unit 2	unit 3	unit 4	WPT 1	WPT 2	end of pipe treatment
FW	\$39,000	\$76,000	\$47,000	\$92,000			
unit 1		\$150,000	\$110,000	\$45,000	\$39,000	\$39,000	\$83,000
unit 2	\$50,000		\$134,000	\$40,000	\$76,000	\$76,000	\$102,500
unit 3	\$180,000	\$35,000		\$42,000	\$47,000	\$47,000	\$98,000
unit 4	\$163,000	\$130,000	\$90,000		\$92,000	\$92,000	\$124,000
WPT 1	\$39,000	\$76,000	\$47,000	\$92,000			
WPT 2	\$39,000	\$76,000	\$47,000	\$92,000			
EoPT	\$83,000	\$102,500	\$98,000	\$124,000			

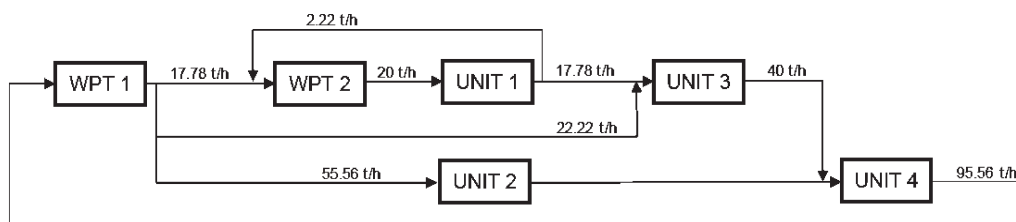


Figure 8. Optimum network of example 8.

Table 16. Water-Using Units Limiting Data of Example 9

process	contaminant	mass load (kg/h)	$C_{in,max}$ (ppm)	$C_{out,max}$ (ppm)
1 steam stripping	HC	0.75	0	15
	H ₂ S	20	0	400
	SS	1.75	0	35
2 HDS-1	HC	3.4	20	120
	H ₂ S	414.8	300	12500
	SS	4.59	45	180
3 desalter	HC	5.6	120	220
	H ₂ S	1.4	20	45
	SS	520.8	200	9500
4 VDU	HC	0.16	0	20
	H ₂ S	0.48	0	60
	SS	0.16	0	20
5 HDS-2	HC	0.8	50	150
	H ₂ S	60.8	400	8000
	SS	0.48	60	120

Table 17. Regeneration Processes Data of Example 9

process	contaminant	removal ratio (%)	OPN _r	VRC _r
1 steam stripping	HC	0	1	16800
	H ₂ S	99.9		
	SS	0		
2 biological treatment	HC	70	0.0067	12600
	H ₂ S	90		
	SS	98		
3 API separator	HC	95	0	4,800
	H ₂ S	0		
	SS	50		

challenges: fixed and variable cost for connection and minimum allowed flow rates through the connections, which makes it a

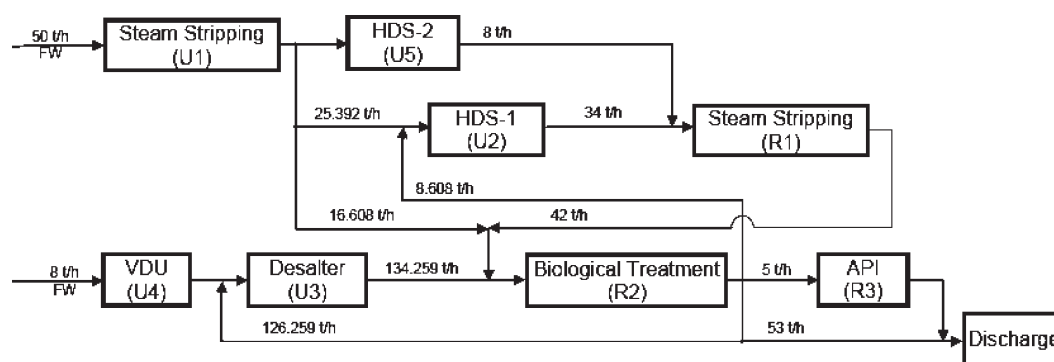
Table 18. Distances for Example 9

d_{ij}	WU 1	WU 2	WU 3	WU 4	WU 5	RG 1	RG 2	RG 3	discharge
FW	30	25	70	50	90	200	500	600	2000
WU 1	0	30	80	150	400	90	150	200	1200
WU 2	30	0	60	100	165	100	150	150	1000
WU 3	80	60	0	50	75	120	90	350	800
WU 4	150	100	50	0	150	250	170	400	650
WU 5	400	165	75	150	0	300	120	200	300
RG 1	90	100	120	250	300	0	125	80	250
RG 2	150	150	90	170	120	125	0	35	100
RG 3	200	150	350	400	200	80	35	0	100

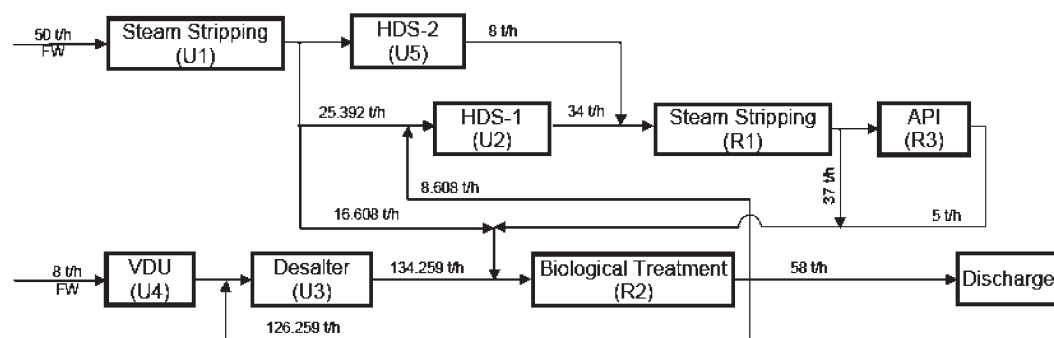
MINLP problem; water-using units with variable flow rates; and, competing regeneration processes (more than one process is able to treat the same contaminant). We assume the minimum flow rate through connection and units is 5 t/h and the maximum is 200 t/h.

BARON solves this problem to global optimality (1% gap) in 25513 s (7 h, 5 m, 13 s), with the minimum TAC of \$574,155. Using the GO method with elimination on discretized variable presented in this section, the lowest time achieved to guarantee the 1% tolerance solution was 25293 CPUs (7 h 1 m 33 s). Incidentally, our wall clock time is 57960 CPUs (16 h 6 m). It is hard to make a meaningful comparison because our code is implemented in GAMS and includes a preprocessing time each time a LB is solved, whereas BARON may skip these steps. Our method analyzes 62 sub problems or passes through the elimination procedure (steps 1 through 7). This procedure used MCP2 with 2 intervals on concentrations and 5 on all flows (units and regeneration processes). Although the presented method takes longer than BARON to find the GO solution, it finds it after bound contraction is performed at the root node. The optimum network found has a TAC of \$578,183, which is higher than and comparable to the one obtained by BARON, but well within the 1% gap. As one can observe in Figure 9, the solutions are similar.

4.10. Comparative Analysis. It seems that using the larger number of intervals possible reduces the number of iterations when the problems are relatively small, which many times do not need any iteration because the solution can be found at the root



(a) Solution obtained by BARON



(b) Our Solution

Figure 9. Optimum networks for example 9.

node. This observation is not necessarily related to the size of the problem, but the tightness of the lower bound model. Note that example 7 and 9 have the same size, however the later showed to be much more difficult to solve for global optimality. The main difference can be attributed to the poor lower bound generated for the latter case. In terms of problem definition, the latter case is a more detailed model than the former. Example 9 assumes water-using units with variable flow rates and also considers cost of connection with a fixed and a variables part, which is what makes the feasible space considerable larger. Degeneracy is also an issue. An analysis of the degenerate solutions of these problems shows that the cost of the solution of example 7 basically depends on the size of the regeneration process. Faria and Bagajewicz²⁴ show that several (at least 50) networks share the same cost, although the number of connections may change. This explains why bound contracting on the regeneration processes flow rates is enough.

Faria and Bagajewicz²⁴ also showed that example 9 has not many degenerate solutions. However, for these, the flow rates through the units and regeneration processes vary, which makes bound contraction difficult. In addition, to further complicate bound contraction procedures, there are several suboptimum solutions (among the first 20 networks) that also make the bound contractions difficult.

Additionally, in some problems we observed that when concentration is discretized, the LB of the *Direct partitioning* is as tight as the *McCormick's envelopes*, and discretization of concentrations normally generates tighter lower bounds than discretization of flow rates.

As a strategy, for large problems, it seems that one should always start increasing the partitioning (larger number of intervals). If the solution is not found with the increase of number of

intervals, an evaluation of the improvement behavior on each of the variables can be performed before it is decided which set of variables should be bound contracted and/or branched.

5. WASTEWATER TREATMENT NETWORKS MODELED AS GENERALIZED POOLING PROBLEMS

Meyer and Floudas²⁵ studied a complex industrial wastewater treatment system as a generalized pooling problem. While pooling problem can be solved using the p-formulation, q-formulation, or pq-formulation, the q-formulation and the pq-formulation becomes quite a challenge for generalized pooling problems because now the proportionality of the pools flow rates has to consider flow rates coming from other pools, which have unknown concentrations. Considering the p-formulation, the generalized pooling problem to solve industrial wastewater systems can be modeled as follows: Given a set of wastewater sources w contaminated by different contaminants c that need to be removed, a set of regeneration processes r with given rate of removal for each contaminant, and a set of disposal sinks s with maximum allowed disposal concentration, one wants to minimize the cost of the wastewater system (Figure 10).

The constraints needed are as follows:

Water Balance of the Wastewater Sources.

$$FW_w = \sum_r FWR_{w,r} + \sum_s FWS_{w,s} \quad \forall w \quad (46)$$

where FW_w is the flow rate from wastewater source w , $FWR_{w,r}$ is the flow rate from wastewater source w to the regeneration process r , and $FWS_{w,s}$ is the flow rate from wastewater source w to the disposal sink s .

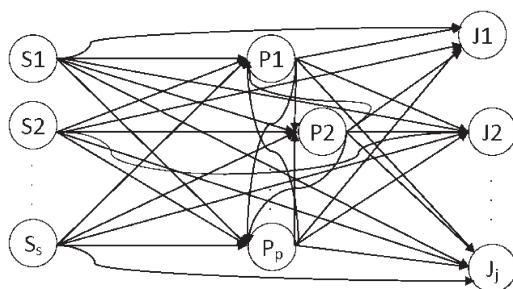


Figure 10. Scheme of the generalized pooling problem.

Water Balance through the Regeneration Processes.

$$FR_r = \sum_w FWR_{w,r} + \sum_{r^*} FRR_{r^*,r} \quad \forall r \quad (47)$$

$$FR_r = \sum_{r^*} FRR_{r,r^*} + \sum_s FRS_{r,s} \quad \forall r \quad (48)$$

where FR_r is the flow rate from regeneration process r , $FRR_{r^*,r}$ is the flow rate from regeneration process r^* to regeneration process r , and $FRS_{r,s}$ is the flow rate from regeneration process r to sink s .

Contaminant Balance at the Regeneration Processes.

$$ZR_{r,c}^{\text{in}} = \sum_w (CW_{w,c} FWR_{w,r}) + \sum_u ZUR_{u,r,c} + \sum_{r^*} ZRR_{r^*,r,c} \quad \forall r, c \quad (49)$$

$$ZR_{r,c}^{\text{out}} = \sum_u ZRU_{r,u,c} + \sum_{r^*} ZRR_{r,r^*,c} + \sum_s ZRS_{r,s,c} \quad \forall r, c \quad (50)$$

where $CW_{w,c}$ is concentration of contaminant c in the wastewater source w , $ZR_{r,c}^{\text{in}}$ is the mass flow of contaminant c going into regeneration process r , and $ZR_{r,c}^{\text{out}}$ is the mass flow of contaminant c leaving regeneration process r .

For the cases in which the regeneration process is assumed to have fixed rate of removal, we use

$$ZR_{r,c}^{\text{out}} = ZR_{r,c}^{\text{in}} (1 - RR_{r,c}) \quad \forall r, c \quad (51)$$

where $RR_{r,c}$ is a given rate of removal of contaminant c in regeneration process r .

Maximum Allowed Discharge Concentration.

$$\sum_w (FWS_{w,s} CW_{w,c}) + \sum_r ZRS_{r,s,c} \leq C_{s,c}^{\text{discharge,max}} \left(\sum_w FWS_{w,s} + \sum_r FRS_{r,s} \right) \quad \forall s, c \quad (52)$$

where $C_{s,c}^{\text{discharge,max}}$ is the maximum allowed concentration at sink s .

Minimum Flow Rates. It is well-known that many solutions of the water problem may include small flow rates that are impractical. To avoid these, we use the following constraints:

$$FWS_{w,s} \geq FWS_{w,s}^{\text{min}} YWS_{w,s} \quad \forall w, s \quad (53)$$

$$FWR_{w,r} \geq FWR_{w,r}^{\text{min}} YWR_{w,r} \quad \forall w, r \quad (54)$$

$$FRR_{r,r^*} \geq FRR_{r,r^*}^{\text{min}} YRR_{r,r^*} \quad \forall r, r^* \quad (55)$$

$$FRS_{r,s} \geq FRS_{r,s}^{\text{min}} YRS_{r,s} \quad \forall r, s \quad (56)$$

$$FR_r \geq FR_r^{\text{min}} YR_r \quad \forall r \quad (57)$$

Table 19. Source Data: Example 13

	W1	W2	W3	W4	W5	W6	W7
flow	20	50	47.5	28	100	30	25
$CW_{w,c1}$	100	800	400	1200	500	50	1000
$CW_{w,c2}$	500	1750	80	1000	700	100	50
$CW_{w,c3}$	500	2000	100	400	250	50	150

These constraints use a set of binary variables ($YWS_{w,s}$, $YWR_{w,r}$, YRR_{r,r^*} , and $YRS_{r,s}$) that are equal to one when the corresponding flow rate is different from zero and zero otherwise.

Maximum Flow Rates. To ensure that the connections do not surpass maximum values, we use the following constraints:

$$FWS_{w,s} \leq FWS_{w,s}^{\text{max}} YWS_{w,s} \quad \forall w, s \quad (58)$$

$$FWR_{w,r} \leq FWR_{w,r}^{\text{max}} YWR_{w,r} \quad \forall w, r \quad (59)$$

$$FRR_{r,r^*} \leq FRR_{r,r^*}^{\text{max}} YRR_{r,r^*} \quad \forall r, r^* \quad (60)$$

$$FRS_{r,s} \leq FRS_{r,s}^{\text{max}} YRS_{r,s} \quad \forall r, s \quad (61)$$

$$FR_r \leq FR_r^{\text{max}} YR_r \quad \forall r \quad (62)$$

The contaminant mass flow rates are enough and no new variables are needed in the case of mixing nodes. However, the splitting nodes at the outlet of each regeneration process need constraints that will reflect that all these contaminant flows and the total mass flows are consistent with the concentrations of the different contaminants. Thus we add the corresponding relations.

Contaminant Mass Flow Rates.

$$ZRR_{r,r^*,c} = FRR_{r,r^*} CR_{r,c}^{\text{out}} \quad \forall r, r^*, c \quad (63)$$

$$ZRS_{r,s,c} = FRS_{r,s} CR_{r,c}^{\text{out}} \quad \forall r, s, c \quad (64)$$

$$ZR_{r,c} = FR_r CR_{r,c}^{\text{out}} \quad \forall r, c \quad (65)$$

where $CR_{r,c}^{\text{out}}$ is the outlet concentration of contaminant c in regeneration r . Finally, we write

$$CR_{r,c}^{\text{out,min}} \leq CR_{r,c}^{\text{out}} \leq CR_{r,c}^{\text{out,max}} \quad \forall r, c \quad (66)$$

Objective Functions. Here the objective function is to minimize the total cost of the system given by

$$TC = \sum_w \left(\begin{aligned} &+ \sum_r (FWRC_{w,r} YWR_{w,r} + VWRC_{w,r} FWR_{w,r}) \\ &+ \sum_s (FWSC_{w,s} YWS_{w,s} + VWSC_{w,s} FWS_{w,s}) \end{aligned} \right) + \sum_r \left(\begin{aligned} &FRC_r YR_r + VRC_r FR_r \\ &+ \sum_{r^*} (FRR_{r,r^*} YRR_{r,r^*} + VRR_{r,r^*} FRR_{r,r^*}) \\ &+ \sum_s (FRS_{r,s} YRS_{r,s} + VRS_{r,s} FRS_{r,s}) \end{aligned} \right) \quad (67)$$

5. GENERALIZED POOLING RESULTS

5.1. Example 10. To illustrate the use of generalized pooling problems, we use the example from Meyer and Floudas.²⁵ The data for this problem is presented in Tables 19 and 20. The discharge limits of this system are 5, 5, and 10 ppm for C1, C2, and C3, respectively. Table 21 shows the distances among

Table 20. Data of Regeneration Processes: Example 13

	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
C1	90	87.5	99	0	90	0	0	99.5	10	70
C2	95	50	90	75	90	0	87	0	99	20
C3	0	50	95	75	20	95	90	0	0	30
FRC _r	48901	36676	13972	48901	48901	48901	36676	36676	13972	13972
VRC _r	3860.3	2895.2	1102.9	3860.3	3860.3	3860.3	2895.2	2895.2	1102.9	1102.9

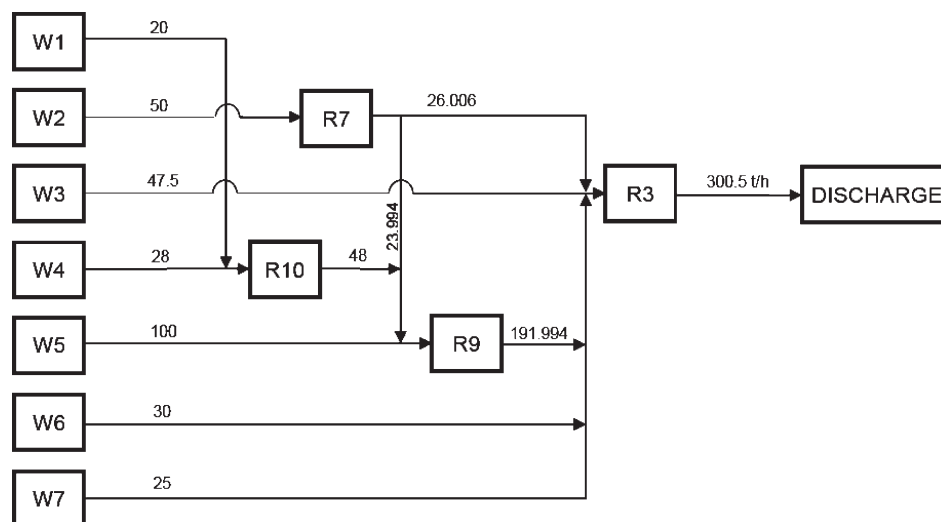


Figure 11. Optimum network of example 13.

Table 21. Distances for Example 13

$d_{i,j}$	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	S1
W1	40	65	75	100	120	110	150	210	280	245	150
W2	15	40	55	75	90	90	125	180	260	215	135
W3	40	35	30	65	100	85	115	170	240	220	100
W4	85	80	55	100	140	120	140	180	245	245	90
W5	95	70	55	45	75	45	40	75	150	150	40
W6	80	70	40	90	125	100	120	150	230	230	70
W7	70	45	30	40	75	50	60	100	175	165	45
R1	-	20	40	50	70	70	100	160	230	190	120
R2	20	-	30	30	60	50	80	140	215	180	95
R3	40	30	-	40	80	60	80	140	210	190	75
R4	50	30	40	-	40	15	50	110	180	150	85
R5	70	60	80	40	-	25	50	110	180	120	120
R6	70	50	60	15	25	-	30	100	170	130	90
R7	100	80	80	50	50	30	-	60	130	100	80
R8	160	140	140	110	110	100	60	-	70	100	95
R9	230	215	210	180	180	170	130	70	-	110	160
R10	190	180	190	150	120	130	100	100	110	-	190

processes. Thus, the piping costs are calculated using eqs 44 and 45.

For this problem, Meyer and Floudas²⁵ present a method to obtain a lower bound, but no systematic procedure to reduce the gap. Their procedure is based on the partition of the feasible region and reformulation. They obtained an upper bound running DICOPT 1000 times with random initial values identifying an answer with a cost of \$1,091,160. They also report that the best known solution has an objective of \$1,086,430, without

citing the source. Using their procedure, they found a lower bound solution 1.2% below the best known solution in 285,449 CPUs (79 h 17 m 29 s). In turn, the best solution found by BARON was \$1,107,905.

Our method renders the network presented in Figure 11, which has a total cost of \$1,086,187. Faria and Bagajewicz²⁴ discuss some additional details regarding computing time. Recently the time reported by Meyer and Floudas²⁵ has been reduced²⁶ considerably (10–20 fold) when using CPLEX 12, which makes their time for one lower bound calculation comparable to our total time obtained using our complete procedure.

6. CONCLUSIONS

We have presented a partitioning-based bound contraction global optimization algorithm for bilinear MINLP problems containing univariate concave functions. We use several different strategies for bound contraction. We applied the strategy to water management problems and the generalized pooling problems. In most cases the performance reported is superior to other methods. In the case of the generalized pooling example, our solution is, to our knowledge, the first global optimum obtained using a systematic procedure. We also looked into wastewater systems modeled as generalized pooling problems, showing that the method can solve them in a time similar to which other approaches take to solve just one lower bound.

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NOMENCLATURE

FWU_{w,u} = flow rate from freshwater source w to the unit u
 FUU_{u*,u} = flow rates between units u^* and u
 FRU_{r,u} = flow rate from regeneration process r to unit u
 FUS_{u,s} = flow rate from unit u to sink s
 FUR_{u*,r} = flow rate from unit u to regeneration process r
 FWR_{w,r} = flow rate from freshwater source w to the regeneration process r
 FRR_{r*,r} = flow rate from regeneration process r^* to regeneration process r
 FRS_{r,s} = flow rate from regeneration process r to sink s
 CW_{w,c} = Concentration of contaminant c in the freshwater source w
 $\Delta M_{u,c}$ = mass load of contaminant c extracted in unit u
 ZUU_{u*,u,c} = mass flow of contaminant c in the stream leaving unit u^* and going to unit u
 ZRU_{r,u,c} = mass flow of contaminant c in the stream leaving regeneration process r and going to unit u
 ZUS_{u,s,c} = mass flow of contaminant c in the stream leaving unit u and going to sink s
 ZUR_{u,r,c} = mass flow of contaminant c in the stream leaving unit u and going to regeneration process r
 $C_{u,c}^{\text{in,max}}$ = maximum allowed concentration of contaminant c at the inlet of unit u
 $C_{u,c}^{\text{out,max}}$ = maximum allowed concentration of contaminant c at the outlet of unit u
 ZR_{r,c}^{\text{in}}} = mass flow of contaminant c going into regeneration process r
 ZR_{r,c}^{\text{out}}} = mass flow of contaminant c leaving regeneration process r
 CRF_{r,c}^{\text{out}}} = outlet concentration of contaminant c in regeneration process r
 XCR_{r,c} = binary parameter that indicates if contaminant c is treated by regeneration process r
 RR_{r,c} = rate of removal of contaminant c in regeneration process r
 CAP_r = capacity of regeneration process r
 $C_{s,c}^{\text{discharge,max}}$ = maximum allowed concentration at sink s
 YWU_{w,u} = binary variable to define the existence of a connection between freshwater source w and unit u
 YUU_{u,u*} = binary variable to define the existence of a connection between unit u and unit u^*
 YUS_{u,s} = binary variable to define the existence of a connection between unit u and sink s
 YUR_{u,r} = binary variable to define the existence of a connection between unit u and regeneration process r
 YRU_{r,u} = binary variable to define the existence of a connection between regeneration process r and unit u
 YRR_{r,r*} = binary variable to define the existence of a connection between regeneration process r and regeneration process r^*
 YRS_{r,s} = binary variable to define the existence of a connection between regeneration process r and sink s
 $C_{u,c}^{\text{out}}$ = outlet concentration of contaminant c in unit u
 CR_{r,c}^{\text{out}}} = outlet concentration of the not treated contaminant c in regeneration r
 FW = freshwater consumption
 FWU_{w,u} = freshwater from source w consumed by unit u
 FWR_{w,r} = freshwater from source w consumed by regeneration process r

TAC = the total annual cost
 OPN_r = operational cost of the regeneration processes
 OP = hours of operation per year
 af = annualization factor
 N = number of years of depreciation
 CCR_r = capital cost coefficient of the regeneration processes
 FCI = fixed capital of investment
 FWUC_{w,u} = fixed capital cost of the connection between freshwater source w and unit u
 FWRC_{w,r} = fixed capital cost of the connection between freshwater source w and regeneration process r
 FWSC_{w,s} = fixed capital cost of the connection between freshwater source w and sink s
 FUUC_{u,u*} = fixed capital cost of the connection between freshwater unit u and unit u^*
 FURC_{u,r} = fixed capital cost of the connection between freshwater unit u and regeneration process r
 FUSC_{u,s} = fixed capital cost of the connection between freshwater unit u and sink s
 FRUC_{r,u} = fixed capital cost of the connection between regeneration process r and freshwater unit u
 FRRC_{r,r*} = fixed capital cost of the connection between regeneration process r and regeneration process r^*
 FRSC_{r,s} = fixed capital cost of the connection between regeneration process r and regeneration process r^*
 FRC_r = fixed capital cost of regeneration process r
 VWUC_{w,u} = coefficient of the variable capital cost of the connection between freshwater source w and unit u
 VWRC_{w,r} = coefficient of the variable capital cost of the connection between freshwater source w and regeneration process r
 VWSC_{w,s} = coefficient of the variable capital cost of the connection between freshwater source w and sink s
 VUUC_{u,u*} = coefficient of the variable capital cost of the connection between freshwater unit u and unit u^*
 VURC_{u,r} = coefficient of the variable capital cost of the connection between freshwater unit u and regeneration process r
 VUSC_{u,s} = coefficient of the variable capital cost of the connection between freshwater unit u and sink s
 VRUC_{r,u} = coefficient of the variable capital cost of the connection between regeneration process r and freshwater unit u
 VRRC_{r,r*} = coefficient of the variable capital cost of the connection between regeneration process r and regeneration process r^*
 VRSC_{r,s} = coefficient of the variable capital cost of the connection between regeneration process r and regeneration process r^*
 VRC_r = coefficient of the variable capital cost of regeneration process r
 d_{ij} = distance between two processes
 FW_w = flow rate from wastewater source w
 FR_r = flow rate from regeneration process r
 TC = total cost

REFERENCES

- (1) Faria, D.; Bagajewicz, M. A new approach for global optimization of a class of MINLP problems with applications to water management and pooling problems. *AIChE J.*
- (2) Karupiah, R.; Grossmann, I. E. Global optimization for the synthesis of integrated water systems in chemical processes. *Comput. Chem. Eng.* **2006**, *30*, 650–673.
- (3) McCormick, G. P. Computability of global solutions to factorable nonconvex programs. Convex underestimating problems. *Math. Program.* **1976**, *10* (1), 147–175.

- (4) Zamora, J. M.; Grossmann, I. E. A branch and contract algorithm for problems with concave univariate, bilinear and linear fractional terms. *J. Global Optim.* **1999**, *14*, 217–249.
- (5) Karupiah, R.; Grossmann, I. E. Global optimization of multi-scenario mixed integer nonlinear programming models arising in the synthesis of integrated water networks under uncertainty. *Comput.-Aided Chem. Eng.* **2006**, *21* (2), 1747–1752.
- (6) Bergamini, M. L.; Aguirre, P.; Grossmann, I. Logic based outer approximation for global optimization of synthesis of process networks. *Comput. Chem. Eng.* **2005**, *29*, 1914.
- (7) Bergamini, M. L.; Grossmann, I.; Scenna, N.; Aguirre, P. An improved piecewise outer-approximation algorithm for the global optimization of MINLP models involving concave and bilinear terms. *Comput. Chem. Eng.* **2008**, *32*, 477–493.
- (8) Padberg, M. Approximating separable nonlinear functions via mixed zero-one programs. *Oper. Res. Lett.* **2000**, *27*, 1–5.
- (9) Meyer, C. A.; Floudas, C. A. Global optimization of a combinatorially complex generalized pooling problem. *AIChE J.* **2006**, *52* (3), 1027–1037.
- (10) Savelski, M.; Bagajewicz, M. On the use of linear models for the design of water utilization systems in refineries and process plants. *Chem. Eng. Res. Des.* **2001**, *79*, 600–610.
- (11) Koppol, A. P. R.; Bagajewicz, J. M.; Dericks, B. J.; Savelski, M. J. On zero water discharge solutions in process industry. *Adv. Environ. Res.* **2003**, *8*, 151–171.
- (12) Gunaratnam, M.; Alva-Argaez, A.; Kokosis, A.; Kim, J. K.; Smith, R. Automated design of total water systems. *Ind. Eng. Chem. Res.* **2005**, *44*, 588–599.
- (13) Hallale, N.; Fraser, D. M. Capital cost targets for mass exchange networks. A special case: Water minimization. *Chem. Eng. Sci.* **1998**, *53* (2), 293–313.
- (14) Alva-Argaez, A.; Kokosis, A. C.; Smith, R. A conceptual decomposition of MINLP models for the design of water-using systems. *Int. J. Environ. Pollut.* **2007**, *29*, 177–205.
- (15) Faria, D. C.; Bagajewicz, M. J. Retrofit of water networks in process plants. *Proceedings of the XXII Interamerican Congress of Chemical Engineering*, Buenos Aires, Argentina; 2006.
- (16) Lim, S. R.; Park, D.; Lee, D. S.; Park, J. M. Economic evaluation of water network system through the net present value method based on cost and benefits estimations. *Ind. Eng. Chem. Res.* **2006**, *45*, 7710–7718.
- (17) Lim, S. R.; Park, D.; Park, J. M. Synthesis of an economically friendly water system by maximizing net present value. *Ind. Eng. Chem. Res.* **2007**, *46*, 6936–6943.
- (18) Wan Alwi, S. R.; Manan, Z. A. SHARPS: A new cost-screening technique to attain cost-effective minimum water network. *AIChE J.* **2006**, *52*, 3981–3988.
- (19) Wan Alwi, S. R.; Manan, Z. A.; Samingin, M. H.; Misran, N. A holistic framework for design of cost-effective minimum water utilization network. *J. Environ. Manage.* **2007**.
- (20) Faria, D. C.; Bagajewicz, M. J. Profit-based grassroots design and retrofit of water networks in process plants. *Comput. Chem. Eng.* **2009**, *33* (2), 436–453.
- (21) Faria, D. C.; Bagajewicz, M. J. On the appropriate modeling of the process plant water systems. *AIChE J.* **2010**, *56* (3), 668–689.
- (22) Wang, Y. P.; Smith, R. Wastewater minimization. *Chem. Eng. Sci.* **1994**, *49* (7), 981–1006.
- (23) Kuo, W. C. J.; Smith, R. Effluent treatment system design. *Chem. Eng. Sci.* **1997**, *52* (23), 4273.
- (24) Faria, D.; Bagajewicz, M. On the degeneracy of the water/wastewater allocation problem in process plants. *Ind. Eng. Chem. Res.* **2010**, *49* (9), 4340–4351.
- (25) Meyer, C. A.; Floudas, C. A. Global optimization of a combinatorially complex generalized pooling problem. *AIChE J.* **2006**, *52* (3), 1027–1037.
- (26) Floudas, C. A. Personal communication, 2010.