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Global Optimization Based on Subspaces Elimination: Applications to Generalized Pooling and Water Management Problems

Débora C. Faria and Miguel J. Bagajewicz
Dept. of Chemical Engineering, University of Oklahoma, Norman, OK 73019

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A global optimization strategy based on the partition of the feasible region in boxed subspaces defined by the partition of specific variables into intervals is described. Using a valid lower bound model, we create a master problem that determines several subspaces where the global optimum may exist, disregarding the others. Each subspace is then explored using a global optimization methodology of choice. The purpose of the method is to speed up the search for a global solution by taking advantage of the fact that tighter lower bounds can be generated within each subspace. We illustrate the method using the generalized pooling problem and a water management problem, which is a bilinear problem that has proven to be difficult to solve using other methods. © 2011 American Institute of Chemical Engineers *AIChE J,* 58: 2336–2345, 2012
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Introduction

In this article, we introduce a new strategy to solve nonconvex problems to global optimality. This strategy is based on obtaining subspaces where the global optimum can exist, disregarding the others. Special strategies to investigate each subspace are discussed.

Several different approaches for Global optimization exist. A comprehensive overview of these methodologies can be found in several paper reviews[1–4] and books: Horst and Tuy[5] or Hansen and Walster.[6]

In this article, we present a new methodology that is based on the partitioning of certain (not all) variables to create several boxes. Later, we performed a bound reduction on these variables and proceed to investigate for global optimization, only those subspaces that potentially contain the global optimum.

Our methodology can use many different lower bound and upper bound models. In particular, to solve our examples (the generalized pooling problem presented by Meyer and Floudas[7] and the water management problem by Alva-Argáez et al.[8]), we use the LB model and partitioning method presented by Faria and Bagajewicz.[9] The example was selected because it is difficult to solve, which is also discussed by Faria and Bagajewicz.[9]

The article is organized as follows: We first discuss the methodology. Then, we present the problems that we are going to use to illustrate the method, their models and the results.

Correspondence concerning this article should be addressed to M. J. Bagajewicz at bagajewicz@ou.edu.

Methodology

Consider the following MINLP problem

$$\underset{x,y,K}{\mathrm{Min}} f(x,y,K) \tag{1}$$

s.t

$$g(x,y,K) \leq 0 \tag{2}$$

$$x_i^L \leq x_i \leq x_i^U \quad \forall i = 1,...,m_x \tag{3}$$

$$y_i^L \leq y_i \leq y_i^U \quad \forall j = 1,...,m_y \tag{4}$$

$$x \in R^{m_x}, \quad y \in R^{m_y}, \quad K \in \{0,1\}^{m_K} \tag{5}$$

In this problem the continuous variables are separated in two sets, the set of "space partitioning variables" $X = \{x_i\}$ and the rest of the variables $Y = \{y_i\}$.

We now define the partitions of variables in X as follows

$$\hat{x}_{i,d_i^x} = x_i^L + \left(d_i^x - 1\right)\frac{\left(x_i^U - x_i^L\right)}{D_i^x - 1} \quad \forall x_i \in X, d_i^x = 1,...,D_i^x \tag{6}$$

Now that the partitioned intervals have been defined, the following constraints force the variables x_i to be in one and only one partition

$$\sum_{d_i^x=1}^{D_i^x-1} \hat{x}_{i,d_i^x}\,\lambda_{i,d_i^x} \leq x_i \leq \sum_{d=1}^{D_i^x-1} \hat{x}_{i,d_i^x+1}\,\lambda_{i,d_i^x} \quad \forall x_i \in X \tag{7}$$

$$\sum_{d_i^x=1}^{D_i^x-1} \lambda_{i,d_i^x} = 1 \quad \forall i = 1,...,m_x \tag{8}$$

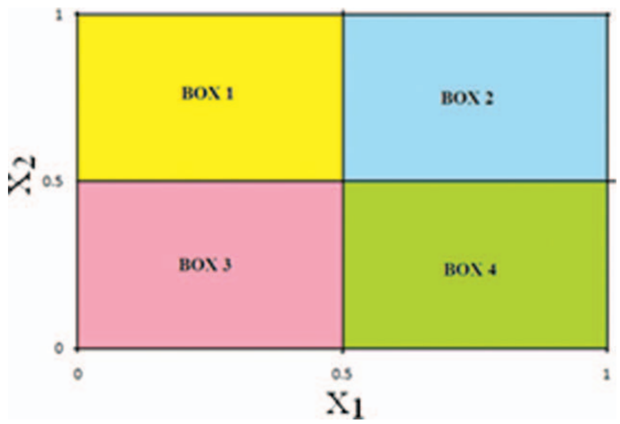

Figure 1. Subspace of the partition variable.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

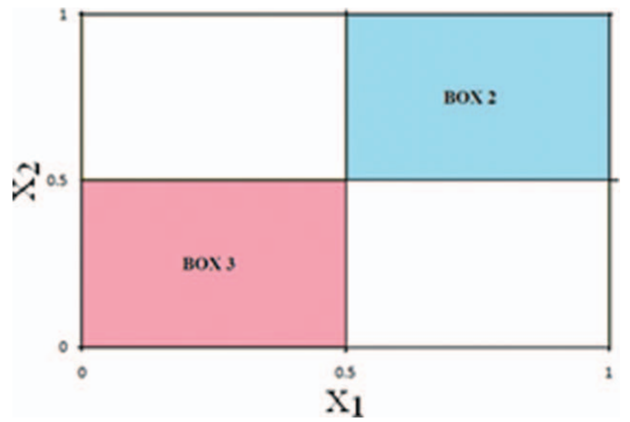

Figure 2. Illustration of surviving subspaces (boxes 2 and 3).

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where variables ${\lambda_{i,d_i}}^x$ are binary. The set of all binaries is called Λ and clearly $\Lambda \in \{0,1\}^{\sum_{i=1,\ldots,m_x} D_i^x}$, that is, it contains all the binaries for all the variables in X and all their partitions. Incidentally, Eqs. 7 and 8 are a subset of several partitioning procedures (see Faria and Bagajewicz[9] for a discussion), and although they are used to obtain lower bounds, they also play an additional role for subspace elimination.

Consider now that a lower bound model of the original problem is constructed. Such a model is usually an MILP model obtained by performing certain relaxations of the different terms in the objective function and constraints. When constraints (7) and (8) are added to this LB model, we call this model LB^0. We note that such a LB model is not necessarily linear, but it is the usual case. For example, when g(x,y,K) is bilinear in the continuous variables, the lower bound is MILP, which was discussed in detail by Faria and Bagajewicz.[9]

Assume now that LB^0 is solved and a certain solution (x^0, y^0, K^0, Λ^0) is obtained. We now say we have identified our first subspace $\Omega^{(0)}$ by writing $\Omega^{(0)} = \Lambda^0$, which is associated to a set of boxes (partitions) defined by $\Omega^{(0)}_{i,dix} = {\lambda_{i,d_i^x}}^0$. We note that the boxes (partitions) formally extend to ALL variables in X. If we want to identify another lower bound and its associated subspace $\Omega^{(1)}$ (different from $\Omega^{(0)}$), we add the following well-known integer cut

$$\sum_{d_i^x=1,\ldots,D_i^x} \Omega^{(0)}_{i,d_i^x} \lambda_{i,d_i^x} \leq \left(\sum_{d_i^x=1,\ldots,D_i^x} \Omega^{(0)}_{i,d_i^x} \right) - 1 \quad \forall i = 1,\ldots,m_x \tag{9}$$

When this constraint is added to the lower bound model, we call this problem LB-MASTER$^{(1)}$. Generalizing, we define problem LB-MASTER$^{(r)}$ as the optimization problem defined by LB^0 and the following additional constraints

$$\sum_{d_i^x=1,\ldots,D_i^x} \Omega^{(r)}_{i,d_i^x} \lambda_{i,d_i^x} \leq \left(\sum_{d_i^x=1,\ldots,D_i^x} \Omega^{(r)}_{i,d_i^x} \right) - 1 \quad \forall i = 1,\ldots,m_x; \forall r = 1,\ldots,t-1 \tag{10}$$

where $\Omega^{(\mathrm{r})}_{i,dx,i}$ is a vector of optimal values of λ_{i,d_i^x} for the rth problem.

Thus, if LB-MASTER$^{(r)}$ is run recursively one can construct a sequence of different subspaces of the partition variables, namely$\{\Omega^{(0)}, \Omega^{(1)}, \ldots, \Omega^{(t)}\}$. This sequence stops at iteration t, when the gap between the LB and any known UB becomes negative (that is, LB>UB).

We illustrate the concept graphically for a very simple problem of two partition variables. Figure 1 shows 4 boxes corresponding to the partition variables x_1 and x_2.

Assume, now that the lower bound model is run, and box 2 is identified as optimal. Assume further that box 3 is identified as the second lower bound. Finally assume that the third problem gives a solution with negative gap. Thus, only two subspaces have been identified as potentially containing the global optimum. This is shown in Figure 2.

Suppose now that after running this problem, only boxes 2 and 4 are identified as the ones possibly containing the global optimum, as shown in Figure 3.

This means that boxes 1 and 3 fathom and one can perform a bound contraction on variable x_1. We call this "bound contraction through subspace fathoming." Although this is a bound contraction method in which several variables may be contracted at the same time, it should not be confused with other bound contraction methodologies,[9–12] where the bound contraction takes place one variable at a time. In

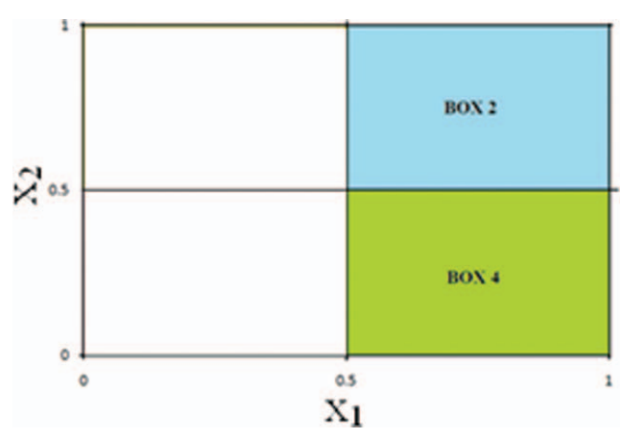

Figure 3. Illustration of surviving subspaces (boxes 2 and 4).

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reality Ryoo and Sahinidis[10] call their procedure "range reduction technique," which together with a branch and bound framework creates the "branch-and-reduce" algorithm. Their range contraction is done adding inequalities constructed with the dual multiplier of active constraints (or variables). So indirectly they could be contracting the bounds of more than one variable at a time, but this is not explicit. Finally, the above procedure falls somehow as under the description of a general prototype of a branch and bound algorithm offered by Horst and Tuy.[5]

We propose several variants of procedures whose efficiency we explore:

Subspace Enumeration First. In this procedure, we identify all boxes, one after another. The procedure is the following:

(1) Run the Lower Bound model and use the solution as starting point for the NLP (or MINLP) original model.

(2) (Optional) Perform bound contraction. Note that any bound contraction procedure can be used. In our example, we use the one presented by Faria and Bagajewicz.[9]

(3) Set $r = 0$

(4) Run the LB-MASTER$^{(r)}$ model.

(5) If the LB is higher than the current global UB, go to step 10.

(6) Use the solution of the LB model as a starting point of the upper bound model, thus (eventually) obtaining a new updated global UB.

(7) Run the LB model again confining the partition variables to the current selected box. We call this LB_r. If LB_r is larger than the current global UB, fathom the present box. Likewise, fathom all previous boxes for which LB_r is larger than the current updated global upper bound.

(8) (Optional) Run the UB model confining all variables to the box found. At this point one can use the box for partition variables only, or even add the box for the partitioned variables. The aim here is to obtain a better upper bound when step 6 failed to produce a feasible solution. If the UB model is too time consuming, one can omit this step, if step 6 produced a feasible point.

(9) Add an integer cut to remove the current subspace from consideration. Set $r=r+1$ and go to step 4.

(10) Fathom all boxes for which LB_r is higher than the new UB. Perform bound contraction through subspace fathoming. If bound contraction is possible, update the bounds, partition the space again, and go to step 3. Otherwise go to step 11.

(11) Pick the box with the smallest LB_r. Attempt global optimization inside this box, considering the current global UB when the UB is updated. The search should stop when the local LB is higher than the global UB.

(12) If no new box is available, stop. The Global Optimum was found.

Global Optimization Inside Each Subspace First. In this procedure, we identify all boxes and seek the global optimum in each box before we proceed to the next. The procedure is:

(1) Run the Lower Bound model and use the solution as starting point for the NLP (or MINLP) original model.

(2) (Optional) Perform bound contraction. Note that any bound contraction procedure can be used. In our example, we use the one presented by Faria and Bagajewicz.[9]

(3) Set $r = 0$.

(4) Run the LB-MASTER$^{(r)}$ model.

(5) If the LB is higher than the current global UB, Stop.

(6) Use the solution of the LB model as a starting point of the upper bound model, thus (eventually) obtaining a new updated global UB.

(7) Obtain the global optimum inside the current box. Update the global UB if needed. In this step, any global optimization method can be used. Any update of the UB should consider the current global UB.

(8) Set $r = r+1$ and go to step 4.

The choice of what variable should be partitioned is related to the improvement of the objective function of the LB-MASTER$^{(r)}$ when subspaces are forbidden. This can be heuristically done choosing different alternatives and analyzing the improvement or, it can be systematically done using information from the Lagrangean multipliers obtained in the lower bound solution of the first master problem (without any forbidden subspace). The higher the Lagrangean multiplier is, the more likely the objective function will increase with changes in the bounds. We do not use this method in this article.

Although there are several other options, the algorithm we chose for obtaining the global optimum at each instance needed in the above procedure is the one implemented by Faria and Bagajewicz.[9] Summarizing, the algorithm is summarized as follows:

- Construct a lower bound model. For bilinear cases, we partition variables in bilinear and quadratic terms, thus relaxing 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 that are to be bound contracted. These variables need not be the same variables as the ones using to construct the lower bound.
- Based on this information the value of the upper bound found by running the original MINLP using the information obtained by solving the lower bound model to obtain a good starting point.
- If the objective function gap between the upper bound solution and the lower bound solution is lower than the tolerance, the solution was found. Otherwise go to the next step.
- If the new problem is infeasible, or if feasible but the objective function is higher than the current upper bound, then all the intervals that have not been forbidden for this variable are eliminated. The surviving feasible region between the new bounds is partitioned again.
- Repeat the last 2 steps for all the other variables, one at a time.
- Go back to the first step (a new iteration using contracted bounds starts).
- Different options for bound contracting have been proposed[9]: One-pass interval elimination, cyclic elimination, single and extended interval forbidding, etc., all of which are detailed in the article referenced.
- 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 the partitioning of the variables to a level in which the sizes of the intervals are small enough to generate a lower bound within a given acceptable tolerance to the upper bound; or,
    - Recursively split the problem in two or more subproblems using a strategy such as the ones based on branch and bound procedure.

Note that to guarantee the optimality, not all of the lower bound models need to be solved to zero gap. The only problems that need to have zero gap are the ones in which the lower bound of the problem (or subproblems) are obtained, which is done in the first step. The LB models used to eliminate intervals can be solved to feasibility between its lower bound and the current upper bound, which is set as the UB of the whole procedure.

The special case of bilinear MINLP problems

We now address in more detail how to apply the above method to the case of bilinear MINLP problems. For completeness, we define the set Y as a union of three sets: $X \cup Y = V \cup W \cup Z \cup R$. Here $V = \{v_j\}$, $W = \{w_k\}$, $Z = \{z_{j,k}\}$, and $R = \{r_l\}$. Thus, all variables participating in bilinear terms are included in V, W, and Z, and the rest, in R. Thus

$$z_{j,k} = v_j w_k \quad \forall j,k \tag{11}$$

The use of partitioning of certain variables to generate valid lower bounds is a common practice in global optimization. In our previous paper,[9] we discuss different partitioning methods as well as present a new bound contraction procedure. Thus it is common practice to partition one of the variables, say v_j. Thus, the lower bound model LB^0 can be constructed partitioning X and V.

It is important to notice that X and V need not have an empty intersection. In fact, all variants for X can be chosen as completely separate from Y. As stated above, that is $X \cap Y = \phi$, or $X=R$ or a subset of R, $X=V$ or a subset of V, $X=W$ or a subset of W or any combination thereof. In particular, when $X=V$, the analysis of the subspaces directly affects the tightness of the lower bound model due to the automatic contractions of the bounds of the partitioned variables.

Illustrations

We illustrate our methodology using the generalized pooling problem applied to a wastewater treatment subsystem and to an industrial water management problem.

Generalized pooling example

The generalized pooling problem differs from the regular pooling problem because it allows connections between elements of the same set, in this case, the pools.

Although pooling problems can be solved using the *p*-formulation, the *q*-formulation or the *pq*-formulation in the case of the generalized pooling problem, the *q*-formulation and *pq*-formulation become a challenge due the fact that now the proportionality of the pools flowrates has to consider flowrates coming from other pools, which have unknown concentrations. This problem was investigated by Meyer and Floudas,[7] which was applied to a complex industrial wastewater treatment system. The generalized pooling problem for industrial wastewater systems is defined 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.

We summarize the *p*-formulation model next, by just stating the equations and referring the reader to the nomenclature section for each variable:

Water balance of the wastewater sources

$$\mathrm{FW}_w = \sum_w \mathrm{FWR}_{w,r} + \sum_s \mathrm{FWS}_{w,s} \quad \forall w \tag{12}$$

Water balance through the regeneration processes

$$\mathrm{FR}_r = \sum_w \mathrm{FWR}_{w,r} + \sum_{r^*} \mathrm{FRR}_{r^*,r} \quad \forall r \tag{13}$$

$$\mathrm{FR}_r = \sum_{r^*} \mathrm{FRR}_{r,r^*} + \sum_s \mathrm{FRS}_{r,s} \quad \forall r \tag{14}$$

Contaminant balance at the regeneration processes

$$\mathrm{ZR}^{\mathrm{in}}_{r,c} = \sum_w \left(\mathrm{CW}_{w,c}\ \mathrm{FWR}_{w,r}\right) + \sum_{r^*} \mathrm{ZRR}_{r^*,r,c} \quad \forall r,c \tag{15}$$

$$\mathrm{ZR}^{\mathrm{out}}_{r,c} = \sum_{r^*} \mathrm{ZRR}_{r,r^*,c} + \sum_s \mathrm{ZRS}_{r,s,c} \quad \forall r,c \tag{16}$$

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

$$\mathrm{ZR}^{\mathrm{out}}_{r,c} = \mathrm{ZR}^{\mathrm{in}}_{r,c}\left(1 - \mathrm{RR}_{r,c}\right) \quad \forall r,c \tag{17}$$

Maximum allowed discharge concentration

$$\sum_w \left(\mathrm{FWS}_{w,s}\mathrm{CW}_{w,c}\right) + \sum_r \mathrm{ZRS}_{r,s,c} \le C^{\mathrm{discharge,max}}_{s,c} \times \left(\sum_w \mathrm{FWS}_{w,s} + \sum_r \mathrm{FRS}_{r,s}\right) \quad \forall s,c \tag{18}$$

Minimum flowrates

$$\mathrm{FWS}_{w,s} \ge \mathrm{FWS}^{\mathrm{Min}}_{w,s}\mathrm{YWS}_{w,s} \quad \forall w,s \tag{19}$$

$$\mathrm{FWR}_{w,r} \ge \mathrm{FWR}^{\mathrm{Min}}_{w,r}\mathrm{YWR}_{w,r} \quad \forall w,r \tag{20}$$

$$\mathrm{FRR}_{r,r^*} \ge \mathrm{FRR}^{\mathrm{Min}}_{r,r^*}\mathrm{YRR}_{r,r^*} \quad \forall r,r^* \tag{21}$$

$$\mathrm{FRS}_{r,s} \ge \mathrm{FRS}^{\mathrm{Min}}_{r,s}\mathrm{YRS}_{r,s} \quad \forall r,s \tag{22}$$

$$\mathrm{FR}_r \ge \mathrm{FR}^{\mathrm{Min}}_r\mathrm{YR}_r \quad \forall r \tag{23}$$

Maximum flowrates

$$\mathrm{FWS}_{w,s} \le \mathrm{FWS}^{\mathrm{Max}}_{w,s}\mathrm{YWS}_{w,s} \quad \forall w,s \tag{24}$$

$$\mathrm{FWR}_{w,r} \le \mathrm{FWR}^{\mathrm{Max}}_{w,r}\mathrm{YWR}_{w,r} \quad \forall w,r \tag{25}$$

$$\mathrm{FRR}_{r,r^*} \le \mathrm{FRR}^{\mathrm{Max}}_{r,r^*}\mathrm{YRR}_{r,r^*} \quad \forall r,r^* \tag{26}$$

$$\mathrm{FRS}_{r,s} \le \mathrm{FRS}^{\mathrm{Max}}_{r,s}\mathrm{YRS}_{r,s} \quad \forall r,s \tag{27}$$

$$\mathrm{FR}_r \le \mathrm{FR}^{\mathrm{Max}}_r\mathrm{YR}_r \quad \forall r \tag{28}$$

Contaminant mass flowrates

$$\mathrm{ZRR}_{r,r^*,c} = \mathrm{FRR}_{r,r^*}\mathrm{CR}^{\mathrm{out}}_{r,c} \quad \forall r,r^*,c \tag{29}$$

$$\mathrm{ZRS}_{r,s,c} = \mathrm{FRS}_{r,s}\mathrm{CR}^{\mathrm{out}}_{r,c} \quad \forall r,s,c \tag{30}$$

Table 1. Sources Data

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

$$ZR_{r,c} = FR_r CR^{out}_{r,c} \quad \forall r, c \tag{31}$$

Finally, we write

$$CR^{out,Min}_{r,c} \leq CR^{out}_{r,c} \leq CR^{out,Max}_{r,c} \quad \forall r, c \tag{32}$$

Objective function

$$TC = \sum_w \begin{pmatrix} +\sum_r \left(FWRC_{w,r}\, YWR_{w,r} + VWRC_{w,r}\, FWR_{w,r}\right) \\ +\sum_s \left(FWSC_{w,s}\, YWS_{w,s} + VWSC_{w,s}\, FWS_{w,s}\right) \end{pmatrix} + \sum_r \begin{pmatrix} FRC_r\, YR_r + VRC_r\, FR_r \\ +\sum_{r^*} \left(FRRC_{r,r^*}\, YRR_{r,r^*} + VRRC_{r,r^*}\, FRR_{r,r^*}\right) \\ +\sum_s \left(FRSC_{r,s}\, YRS_{r,s} + VRSC_{r,s}\, FRS_{r,s}\right) \end{pmatrix} \tag{33}$$

The data for this problem is presented in Tables 1 and 2. The discharge limits of the system are 5 ppm, 5 ppm and 10 ppm for three different contaminants, C1, C2 and C3 respectively.

Table 3 shows the distances among processes, which is used to calculate the piping costs using Eqs. 34 and 35

$$FIJC_{i,j} = 124.6\ d_{i,j} \quad \forall i \in \{W, R\}, j \in \{W, R, S\} \tag{34}$$

$$VIJC_{i,j} = 1.001\ d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \tag{35}$$

Faria and Bagajewicz[9] presented a methodology that is based on partitioning of one of the variables in the bilinear term, which allowed obtaining a lower bound. The partitioning methods presented are variations of earlier work.[11–13] While most work that used partitioning relied on Branch and Bound over the newly created intervals[11,13] as their central procedure, we resort to an interval elimination procedure to perform a novel Bound Contraction method and only resort to a branch and bound procedure when bound contraction does not show any additional progress. In our Branch and Bound procedure, however, we can branch on the nonpartitioned variable instead, since the interval elimination is normally done over the partitioned variable.

We now show the results of the proposed method. Table 4 shows two results found using different partitioning level when applied the global optimization inside each subspace first. Both used the flowrates through the pools (regeneration processes) as the partitioning variables, which creates the boxes. We run this problem by picking the concentrations of the pools and flowrates through the regeneration processes as partitioned variables, as well as the variables to be bound contracted. The optimality gap was set to be 1%. The bounds of the variables were calculated using bound arithmetic, that is, the lowest possible obtained by the provided data.

Both partitioning levels presented in Table 1 found the same solution. The corresponding network is presented in Figure 4 and its total annual cost is $1,086,187.

This problem was also solved by Faria and Bagajewicz[9] using the bound contraction methodology (outlined above), obtaining the same solution. More detailed results are also shown by Faria and Bagajewicz.[14]

Worth noticing, Meyer and Floudas[7] developed a new formulation for the generalized pooling problem using a piecewise linear relaxation that was able to produce a LB with a 1.2% gap in approximately 79 hours. The LB had an objective of 1.073×10^6, which compared well to a best known solution whose objective value was 1.08643×10^6. Our network is the same as the one corresponding to the best objective that Meyer and Floudas[7] report (the origin of which is unknown), but because in the original paper did not report flowrates and concentrations, it is only safe to speculate that they are the same, because our objectives are strikingly similar, but not exactly the same. Meyer and Floudas[7] used an older version of CPLEX, so with the advances that CPLEX has incorporated lately, the 79 hours should reduce significantly. This is indeed the case. Floudas (personal communication) reported a 10-20 fold reduction in time depending on what parameters of their method were used. The 1.2% gap was calculated comparing with the "best-known" upper bound provided by the authors, not by one that one could obtain by running the nonlinear model using the LB solution as starting point or any other ad-hoc procedure. The methodology was considered efficient for this particular case because a good upper bound was known separately and therefore there was no need to try to close the gap. However, if one does not have a good known upper bound solution (in general and for this case study), then it is unclear how efficient the method would be. In fact, one needs a very fast lower bound if one will do branch contracting, We conclude that an effective methodology is still needed to find feasible solution for the problem so that good upper bounds can be generated and then be able to reduce the gap if they are not close.

Water allocation problem

The water allocation problem (WAP) has been widely studied under several assumptions.[8,9,13,14,15–21] In general, this class of problems 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/

Table 2. Data of Regeneration Processes

	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10
$RR_{r,C1}$ (%)	90	87.5	99	0	90	0	0	99.5	10	70
$RR_{r,C2}$(%)	95	50	90	75	90	0	87	0	99	20
$RR_{r,C3}$(%)	0	50	95	75	20	95	90	0	0	30
FRC_r ($)	48,901	36,676	13,972	48,901	48,901	48,901	36,676	36,676	13,972	13,972
VRC_r ($/t)	3860.3	2895.2	1102.9	3860.3	3860.3	3860.3	2895.2	2895.2	1102.9	1102.9

Table 3. Distances Matrix

$d_{i,j}$ (m)	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

wastewater network that globally optimize a chosen objective function.

The model is standard and the corresponding equations are the following (see nomenclature at the end for the variables definition):

Water balance at the water-using units

$$\sum_w \mathrm{FWU}_{w,u} + \sum_{u^* \neq u} \mathrm{FUU}_{u^*,u} + \sum_r \mathrm{FRU}_{r,u} = \sum_s \mathrm{FUS}_{u,s} + \sum_{u^* \neq u} \mathrm{FUU}_{u,u^*} + \sum_r \mathrm{FUR}_{u,r} \quad \forall u \quad (36)$$

Water balance at the regeneration processes

$$\sum_w \mathrm{FWR}_{w,r} + \sum_u \mathrm{FUR}_{u,r} + \sum_{r^*} \mathrm{FRR}_{r^*,r} = \sum_u \mathrm{FRU}_{r,u} + \sum_{r^*} \mathrm{FRR}_{r,r^*} + \sum_s \mathrm{FRS}_{r,s} \quad \forall r \quad (37)$$

Contaminant balance at the water-using units

$$\sum_w \left(\mathrm{CW}_{w,c}\ \mathrm{FWU}_{w,u}\right) + \sum_{u^* \neq u} \mathrm{ZUU}_{u^*,u,c} + \sum_r \mathrm{ZRU}_{r,u,c} + \Delta M_{u,c} = \sum_{u^* \neq u} \mathrm{ZUU}_{u,u^*,c} + \sum_s \mathrm{ZUS}_{u,s,c} + \sum_r \mathrm{ZUR}_{u,r,c} \quad \forall u, c \quad (38)$$

Maximum inlet concentration at the water-using units

$$\sum_w \left(\mathrm{CW}_{w,c}\ \mathrm{FWU}_{w,u}\right) + \sum_{u^* \neq u} \mathrm{ZUU}_{u^*,u,c} + \sum_r \mathrm{ZRU}_{r,u,c} \leq C_{u,c}^{\mathrm{in,max}} \times \left(\sum_w \mathrm{FUW}_{w,u} + \sum_{u^* \neq u} \mathrm{FUU}_{u^*,u} + \sum_r \mathrm{FRU}_{r,u} \right) \quad \forall u, c \quad (39)$$

Maximum outlet concentration at the water-using units

$$\sum_w \left(\mathrm{CW}_{w,c}\ \mathrm{FWU}_{w,u}\right) + \sum_{u^*} \mathrm{ZUU}_{u^*,u,c} + \sum_r \mathrm{ZRU}_{r,u,c} + \Delta M_{u,c} \leq C_{u,c}^{\mathrm{out,max}} \left(\sum_{u^*} \mathrm{FUU}_{u,u^*} + \sum_r \mathrm{FUR}_{u,r} + \sum_{u^*} \mathrm{FUU}_{u,u^*} + \sum_s \mathrm{FUS}_{u,s} \right) \quad \forall u, c \quad (40)$$

Contaminant balance at the regeneration processes

$$\mathrm{ZR}_{r,c}^{\mathrm{in}} = \sum_w \left(\mathrm{CW}_{w,c}\ \mathrm{FWR}_{w,r}\right) + \sum_u \mathrm{ZUR}_{u,r,c} + \sum_{r^*} \mathrm{ZRR}_{r^*,r,c} \quad \forall r, c \quad (41)$$

$$\mathrm{ZR}_{r,c}^{\mathrm{out}} = \sum_u \mathrm{ZRU}_{r,u,c} + \sum_{r^*} \mathrm{ZRR}_{r,r^*,c} + \sum_s \mathrm{ZRS}_{r,s,c}\ \forall r, c \quad (42)$$

For the cases in which the regeneration process is assumed to have fixed outlet concentration of one (or more) contaminants, Eq. 43 is used.

$$\mathrm{ZR}_{r,c}^{\mathrm{out}} = \mathrm{ZR}_{r,c}^{\mathrm{in}} \left(1 - \mathrm{XCR}_{r,c}\right) + \left(\sum_w \mathrm{FWR}_{w,r} + \sum_u \mathrm{FUR}_{u,r} + \sum_{r^*} \mathrm{FRR}_{r^*,r} \right) \mathrm{CRF}_{r,c}^{\mathrm{out}}\ \mathrm{XCR}_{r,c} \quad \forall r, c \quad (43)$$

In the above equation, $XCR_{r,c}$ is a 0-1 parameter that identifies which contaminant is being treated, that is $XCR_{r,c} = 1$ if contaminant c is treated in treatement unit r.

Table 4. Summary of the Options Tried for the Generalized Pooling Problem[7]

LB Model	Partitioning Variables (Boxes)	Variables for Bound Contraction	Variables for Branch and Bound	Time (CPUs)	Feasible Boxes
MCP2-C Concentrations (2 intervals) Reg. flows (2 intervals)					
	Reg. flows (2 intervals)	Concentrations Reg. flow	All flowrates	4 hrs 1 min 38 s	7
	Reg. flows (3 intervals)	Concentrations Reg. flow	All flowrates	4 hrs 44 min 31 s	18

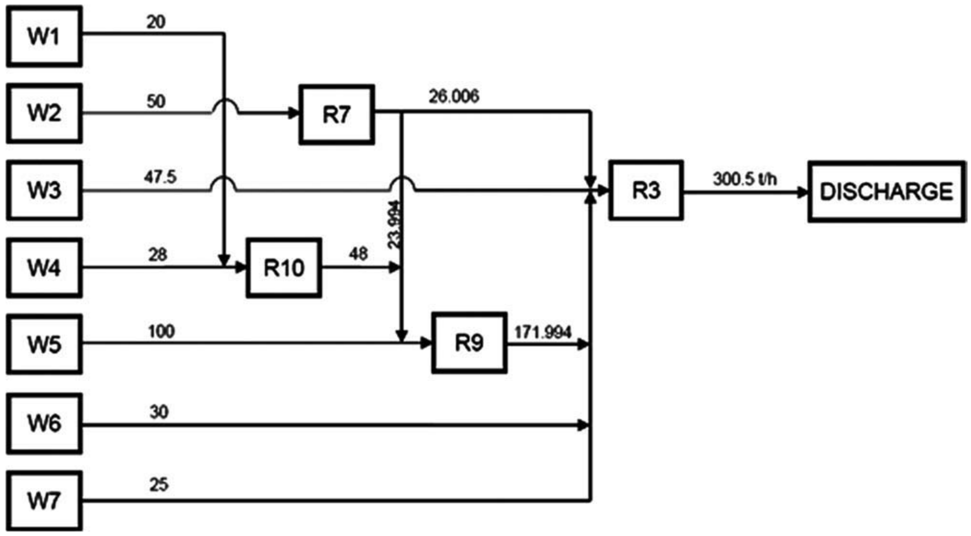

Figure 4. Solution of the generalized pooling problem.

For the cases in which the regeneration process is assumed to have fixed rate of removal, Eq. 44 is used

$$\mathrm{ZR}_{r,c}^{\mathrm{out}} = \mathrm{ZR}_{r,c}^{\mathrm{in}}\left(1 - \mathrm{RR}_{r,c}\right) \quad \forall r, c \tag{44}$$

Capacity of the regeneration processes

$$\mathrm{CAP}_r = \sum_w \mathrm{FWR}_{w,r} + \sum_u \mathrm{FUR}_{u,r} + \sum_{r^*} \mathrm{FRR}_{r^*,r} \quad \forall r \tag{45}$$

Maximum allowed discharge concentration

$$\sum_u \mathrm{ZUS}_{u,s,c} + \sum_r \mathrm{ZRS}_{r,s,c} \le C_{s,c}^{\mathrm{discharge,max}} \times \left(\sum_u \mathrm{FUS}_{u,s} + \sum_r \mathrm{FRS}_{r,s}\right) \quad \forall s, c \tag{46}$$

Minimum flowrates through connections

$$\mathrm{FWU}_{w,u} \ge \mathrm{FWU}_{w,u}^{\mathrm{Min}} \mathrm{YWU}_{w,u} \quad \forall w, u \tag{47}$$

$$\mathrm{FUU}_{u,u^*} \ge \mathrm{FUU}_{u,u^*}^{\mathrm{Min}} \mathrm{YUU}_{u,u^*} \quad \forall u, u^* \tag{48}$$

$$\mathrm{FUS}_{u,s} \ge \mathrm{FUS}_{u,s}^{\mathrm{Min}} \mathrm{YUS}_{u,s} \quad \forall u, s \tag{49}$$

$$\mathrm{FUR}_{u,r} \ge \mathrm{FUR}_{u,r}^{\mathrm{Min}} \mathrm{YUR}_{u,r} \quad \forall u, r \tag{50}$$

$$\mathrm{FRU}_{r,u} \ge \mathrm{FRU}_{r,u}^{\mathrm{Min}} \mathrm{YRU}_{r,u} \quad \forall r, u \tag{51}$$

$$\mathrm{FRR}_{r,r*} \ge \mathrm{FRR}_{r,r*}^{\mathrm{Min}} \mathrm{YRR}_{r,r*} \quad \forall r, r* \tag{52}$$

$$\mathrm{FRS}_{r,s} \ge \mathrm{FRS}_{r,s}^{\mathrm{Min}} \mathrm{YRS}_{r,s} \quad \forall r, s \tag{53}$$

Maximum flowrates through connections

$$\mathrm{FWU}_{w,u} \le \mathrm{FWU}_{w,u}^{\mathrm{Max}} \mathrm{YWU}_{w,u} \quad \forall w, u \tag{54}$$

$$\mathrm{FUU}_{u,u*} \le \mathrm{FUU}_{u,u*}^{\mathrm{Max}} \mathrm{YUU}_{u,u*} \quad \forall u, u* \tag{55}$$

$$\mathrm{FUS}_{u,s} \le \mathrm{FUS}_{u,s}^{\mathrm{Max}} \mathrm{YUS}_{u,s} \quad \forall u, s \tag{56}$$

$$\mathrm{FUR}_{u,r} \le \mathrm{FUR}_{u,r}^{\mathrm{Max}} \mathrm{YUR}_{u,r} \quad \forall u, r \tag{57}$$

$$\mathrm{FRU}_{r,u} \le \mathrm{FRU}_{r,u}^{\mathrm{Max}} \mathrm{YRU}_{r,u} \quad \forall r, u \tag{58}$$

$$\mathrm{FRR}_{r,r*} \le \mathrm{FRR}_{r,r*}^{\mathrm{Max}} \mathrm{YRR}_{r,r*} \quad \forall r, r* \tag{59}$$

$$\mathrm{FRS}_{r,s} \le \mathrm{FRS}_{r,s}^{\mathrm{Max}} \mathrm{YRS}_{r,s} \quad \forall r, s \tag{60}$$

Contaminant mass flowrates

$$\mathrm{ZUU}_{u,u*,c} = \mathrm{FUU}_{u,u*}\, C_{u,c}^{\mathrm{out}} \quad \forall u, u*, c \tag{61}$$

$$\mathrm{ZUS}_{u,s,c} = \mathrm{FUS}_{u,s}\, C_{u,c}^{\mathrm{out}} \quad \forall u, s, c \tag{62}$$

Table 5. Water Using Units Limiting Data of WAP Example

Process	Contaminant	Mass Load (Kg/h)	$C^{\mathrm{in,max}}$ (ppm)	$C^{\mathrm{out,max}}$ (ppm)
(1) Steam stripping	HC	0.75	0	15
	H_2S	20	0	400
	SS	1.75	0	35
(2) HDS-1	HC	3.4	20	120
	H_2S	414.8	300	12,500
	SS	4.59	45	180
(3) Desalter	HC	5.6	120	220
	H_2S	1.4	20	45
	SS	520.8	200	9500
(4) VDU	HC	0.16	0	20
	H_2S	0.48	0	60
	SS	0.16	0	20
(5) HDS-2	HC	0.8	50	150
	H_2S	60.8	400	8000
	SS	0.48	60	120

Table 6. Regeneration Processes Data for the WAP Example

Process	Contaminant	Removal Ratio (%)	OPN_r	VRC_r
(1) Steam stripping	HC	0	1	16,800
	H_2S	99.9		
	SS	0		
(2) Biological treatment	HC	70	0.0067	12,600
	H_2S	90		
	SS	98		
(3) API separator	HC	95	0	4800
	H_2S	0		
	SS	50		

Table 7. Distances for the WAP Example

$d_{i,j}(m)$	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

$$\mathrm{ZUR}_{u,r,c} = \mathrm{FUR}_{u,r}\, C_{u,c}^{\mathrm{out}} \quad \forall u, r, c \tag{63}$$

$$\mathrm{ZRU}_{r,u,c} = \mathrm{FRU}_{r,u}\, \mathrm{CR}_{r,c}^{\mathrm{out}}(1 - \mathrm{XCR}_{r,c}) + \mathrm{FRU}_{r,u}\, \mathrm{CRF}_{r,c}^{\mathrm{out}} \mathrm{XCR}_{r,c} \quad \forall r, u, c \tag{64}$$

$$\mathrm{ZRR}_{r,r^*,c} = \mathrm{FRR}_{r,r^*} \mathrm{CR}_{r,c}^{\mathrm{out}}(1 - \mathrm{XCR}_{r,c}) + \mathrm{FRR}_{r,r^*} \mathrm{CRF}_{r,c}^{\mathrm{out}} \mathrm{XCR}r, c \quad \forall r, r*, c \tag{65}$$

$$\mathrm{ZRS}_{r,s,c} = \mathrm{FRS}_{r,s}\ \mathrm{CR}_{r,c}^{\mathrm{out}}(1 - \mathrm{XCR}_{r,c}) + \mathrm{FRS}_{r,s}\, \mathrm{CRF}_{r,c}^{\mathrm{out}} \mathrm{XCR}_{r,c} \quad \forall r, s, c \tag{66}$$

Minimum and maximum concentrations

$$\mathrm{CR}_{r,c}^{\mathrm{out,Min}} \le \mathrm{CR}_{r,c}^{\mathrm{out}} \le \mathrm{CR}_{r,c}^{\mathrm{out,Max}} \quad \forall r, c \tag{67}$$

$$\mathrm{C}_{u,c}^{\mathrm{out,Min}} \le \mathrm{C}_{u,c}^{\mathrm{out}} \le \mathrm{C}_{u,c}^{\mathrm{out,Max}} \quad \forall u, c \tag{68}$$

Objective functions

Freshwater consumption

$$\mathrm{Min\ FW} = \sum_w \left(\sum_u \mathrm{FWU}_{w,u} + \sum_r \mathrm{FWR}_{w,r} \right) \tag{69}$$

Total Annual Cost

$$\mathrm{Max\ TAC} = \mathrm{OP}\left(\sum_w \alpha_w \left(\sum_u \mathrm{FWU}_{w,m} + \sum_r \mathrm{FWR}_{w,r} \right) + \sum_r \mathrm{OPN}_r \mathrm{FR}_r \right) - af\ \mathrm{FCI} \tag{70}$$

Fixed Capital of Investment

$$\mathrm{FCI} = \sum_w \begin{pmatrix} \sum_u \left(\mathrm{FWUC}_{w,u}\, \mathrm{YWU}_{w,u} + \mathrm{VWUC}_{w,u}\, \mathrm{FWU}_{w,u} \right) \\ + \sum_r \left(\mathrm{FWRC}_{w,r}\, \mathrm{YWR}_{w,r} + \mathrm{VWRC}_{w,r}\, \mathrm{FWR}_{w,r} \right) \\ + \sum_s \left(\mathrm{FWSC}_{w,s}\, \mathrm{YWS}_{w,s} + \mathrm{VWSC}_{w,s}\, \mathrm{FWS}_{w,s} \right) \end{pmatrix} + \sum_u \begin{pmatrix} \sum_{u^*} \left(\mathrm{FUUC}_{u,u^*}\, \mathrm{YUU}_{u,u^*} + \mathrm{VUUC}_{u,u^*}\, \mathrm{FUU}_{u,u^*} \right) \\ + \sum_r \left(\mathrm{FURC}_{u,r}\, \mathrm{YUR}_{u,r} + \mathrm{VURC}_{u,r}\, \mathrm{FUR}_{u,r} \right) \\ + \sum_s \left(\mathrm{FUSC}_{u,s}\, \mathrm{YUS}_{u,s} + \mathrm{VUSC}_{u,s}\, \mathrm{FUS}_{u,s} \right) \end{pmatrix} + \sum_r \begin{pmatrix} \mathrm{FRC}_r\, \mathrm{YR}_r + \mathrm{VRC}_r\, (\mathrm{FR}_r)^{0.7} \\ + \sum_u \left(\mathrm{FRUC}_{r,u}\, \mathrm{YRU}_{r,u} + \mathrm{VRUC}_{r,u}\, \mathrm{FRU}_{r,u} \right) \\ + \sum_{r^*} \left(\mathrm{FRRC}_{r,r^*}\, \mathrm{YRR}_{r,r^*} + \mathrm{VRRC}_{r,r^*}\, \mathrm{FRR}_{r,r^*} \right) \\ + \sum_s \left(\mathrm{FRSC}_{r,s}\, \mathrm{YRS}_{r,s} + \mathrm{VRSC}_{r,s}\, \mathrm{FRS}_{r,s} \right) \end{pmatrix} \tag{71}$$

Connection costs

$$\mathrm{FIJC}_{i,j} = 124.6\ d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \tag{72}$$

$$\mathrm{VIJC}_{i,j} = 1.001\ d_{i,j} \quad \forall i \in \{W, U, R\}, j \in \{W, U, R, S\} \tag{73}$$

To illustrate the method applied for the WAP we solved the refinery case presented by Gunaratna et al.[20] and Alva-Argáez et al.,[8] which minimizes total annual cost considering piping costs as well. Tables 5 and 6 present the data for the processes and the regeneration units. This system operates 8600 hours per year, has freshwater cost of \$0.2/t an discharge limits of 20 ppm for HC, 5 ppm for H_2S and 100 ppm for SS. A 10% rate of discount is assumed.

The distances between processes are presented in Table 7. We assume the minimum flowrate through connection and units is 5 t/h and the maximum is 200 t/h.

Faria and Bagajewicz[9,14] solved this problem for global optimality (1% tolerance) in 25,293 CPUs (7 h 1 m 33 s) finding a TAC of \$578,183. A solution from BARON was also presented, which solves this problem to global

Table 8. Summary of the WAP Solution

LB Model	Partitioning Variables (Boxes)	Variables for Bound Contraction	Variables for Branch and Bound	Time (CPUs)	Feasible Boxes
MCP2-C Concentrations (5 intervals) Reg. flows (2 intervals)					
	Reg. flow (2 intervals)	Concentrations WU flow Reg. flow	All flowrates	10 h 6 m 34 s	4

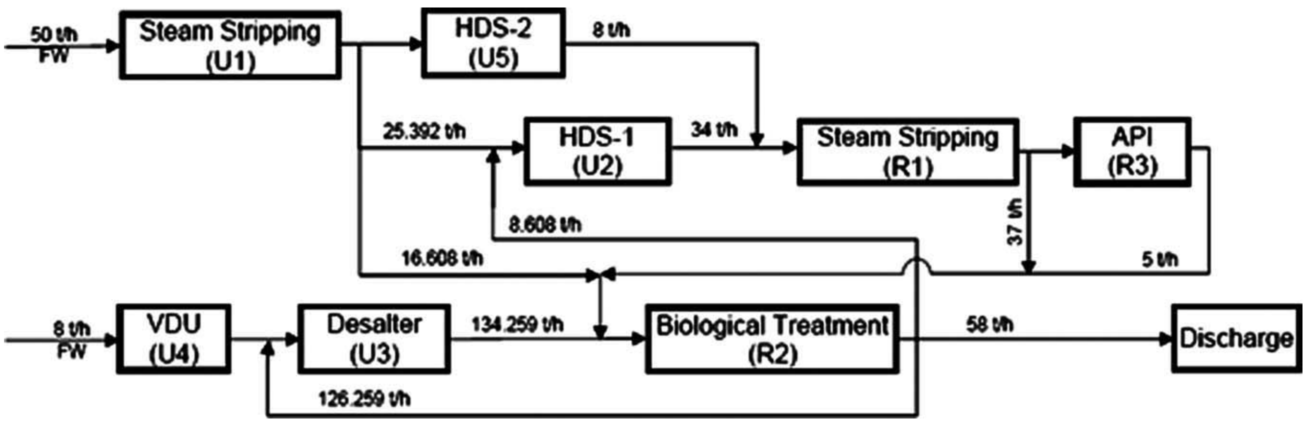

Figure 5. Solution of the WAP.

optimality (1% gap) in 25,513 s (7 h, 5 m, 13 s), with the minimum TAC of $574,155.

For this problem only one strategy is presented (Table 8). Although it did not improve the running time to achieve global optimality, it also converges to the solution. The optimality gap was set to be 1%. Figure 5 presents the network corresponding to the solution, which is the same as the one obtained by Faria and Bagajewicz.[14]

Conclusions

A strategy to globally solve nonconvex problem using a search and elimination of subspaces was presented in this article. The strategy is recommended to large problem where it is difficult (or impossible) to formulate a good (tight) lower bound model.

The strategy has shown some improvement in terms of speed up the search for global optimality of a complex generalized pooling problem. However, there is still a need of systematically define the partitioning variables instead of trying different alternatives. This is a subject for a future work.

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Notation

Generalized Pooling Problem

- FW_w = flowrate from wastewater source w.
- $FWR_{w,r}$ = flowrate from wastewater source w to the regeneration process r.
- $FWS_{w,s}$ = flowrate from wastewater source w to the disposal sink s.
- FR_r = flowrate from regeneration process r,.
- $FRR_{r^*,r}$ = flowrate from regeneration process r^* to regeneration process r.
- $FRS_{r,s}$ = flowrate from regeneration process r to sink s.
- $CW_{w,c}$ = concentration of contaminant c in the wastewater source w
- $ZR^{in}_{r,c}$ = mass flow of contaminant c going into regeneration process r.
- $ZR^{out}_{r,c}$ = mass flow of contaminant c leaving regeneration process r.
- $RR_{r,c}$ = rate of removal of contaminant c in regeneration process r.
- $C^{discharge,max}_{s,c}$ = maximum allowed concentration at sink s.
- $YWS_{w,r}$ = binary variables corresponding to the existence of connection from wastewater source w to sink s.
- $YWR_{w,r}$ = binary variables corresponding to the existence of connection from wastewater source w to regeneration process r.
- YRR_{r,r^*} = binary variables corresponding to the existence of connection from regeneration process r to regeneration process r^*.
- $YRS_{r,s}$ = binary variables corresponding to the existence of connection from regeneration process r to sink s.
- $CR^{out}_{r,c}$ = outlet concentration of contaminant c in regeneration r

Water Allocation Problem

- $FWU_{w,u}$ = flowrate from freshwater source w to the unit u.
- $FUU_{u^*,u}$ = flowrates between units u^* and u.
- $FRU_{r,u}$ = from regeneration process r to unit u.
- $FUS_{u,s}$ = flowrate from unit u to sink s.
- $FUR_{u^*,r}$ = flowrate from unit u to regeneration process r.
- $FWR_{w,r}$ = flowrate from freshwater source w to the regeneration process r.
- $FRR_{r^*,r}$ = flowrate from regeneration process r^* to regeneration process r.
- $FRS_{r,s}$ = flowrate 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.
- $C^{in,max}_{u,c}$ = maximum allowed concentration of contaminant c at the inlet of unit u.
- $C^{out,max}_{u,c}$ = maximum allowed concentration of contaminant c at the outlet of unit u.
- ${ZR_{r,c}}^{in}$ = mass flow of contaminant c going into regeneration process r.
- $ZR^{out}_{r,c}$ = mass flow of contaminant c leaving regeneration process r.
- $CRF^{out}_{r,c}$ = pre-defined 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.
- $C^{discharge,max}_{s,c}$ = maximum allowed concentration at sink s.
- $YWUw,u$, YUU_{u,u^*} $YUS_{u,s}$, $YUR_{u,r}$, $YRU_{r,u}$, YRR_{r,r^*} and $YRS_{r,s}$ = binary variables to define the existence of connevtion between processes.
- $C^{out}_{u,c}$ = outlet concentration of contaminant c in unit u.
- $CR^{out}_{r,c}$ = outlet concentration of contaminant c in regeneration r.
- OPN_r = operating cost of the regeneration processes.
- OP = hours of operation per year.

af = factor that annualizes the capital cost (usually $1/N$, where N is the number of years of depreciation).

CCR_r = capital cost coefficient of the regeneration processes.

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