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A new approach for the design of multicomponent water/wastewater networks

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Abstract

Water allocation problems have nonlinearities and non-convexities due to bilinear terms. To address this issue we propose to discretize one of the variable of the bilinear terms. As a result an MILP model is generated, which provides a lower bound. To reduce the gap between this lower bound and the upper bound (a feasible solution found using the original NLP model), an interval elimination procedure is proposed. As a result, the feasible space shrinks after each iteration and the global optimum is identified. We illustrate the methodology for minimum water allocation problems.

Keywords: water networks, multicoponent, bilinearities, discretization, lower bound.

1. Introduction

The design of water/wastewater networks where water is reused and/or regenerated in processes plants is one important problem in industry as it leads to important water and cost savings. To accomplish this task for multicomponent systesm, mathematical programming is needed (Bagajewicz , 2000). The models contain a large number of bi-linear, non-convex terms, which make the identification of a global optimum cumbersome. To overcome this difficulty, some authors have presented methodologies to find feasible solutions for these systems (Bagajewicz et al.,2000; Alva-Argaez et al., 1998,2007; Ullmer et al.,2005). With the exception of the work presented by Karuppiah and Grossmann (2006), no other present a methodology to find the global optimum solution. In this paper we present a new discretization methodology based on an interval elimination procedure that guarantees global optimality. We present the nonlinear model first, followed by a description of the discretization model and the solution procedure. Finally, an example is presented.

2. The Nonlinear Model

Problem statement: Given a set of water using units, freshwater sources, wastewater sink and available regeneration processes with their limiting data, a globally optimum for the freshwater consumption is sought. The corresponding non-liner model to solve this water allocation problem (WAP) written in terms of contaminant mass load is:

Water balance at the water-using units

$$\sum_{w} FWU_{w,u} + \sum_{u^*} FUU_{u^*,u} + \sum_{r} FRU_{r,u} = \sum_{s} FUS_{u,s} + \sum_{u^*} FUU_{u,u^*} + \sum_{r} FUR_{u^*,r} \qquad \forall u \tag{1}$$

FWU, *FUU*, *FRU*, *FRR* and *FUR* are the freshwater to unit, unit to unit, regeneration unit to units, regeneration to regeneration and unit to regeneration flowrates.

Water balance at the regeneration processes

$$\sum_{u} FUR_{u,r} + \sum_{r^*} FRR_{r^*,r} = \sum_{u} FRU_{r,u} + \sum_{r^*} FRR_{r,r^*} + \sum_{u} FRR_{r,u} \qquad \forall r \tag{2}$$

Contaminant balance at the water-using units

$$\begin{aligned}\sum_{w} \left(CW_{w,c} * FW_{w,u}\right) + \sum_{u^*} ZUU_{u^*,u,d} + \sum_{r} ZRU_{r,u,d} + \Delta M_{u,c} \\ = \sum_{u^*} ZUU_{u,u^*,d} + \sum_{s} ZUS_{u,s,d} + \sum_{r} ZUR_{u,r,d} \qquad \forall u, c\end{aligned} \tag{3}$$

$CW_{w,c}$ is the pollutant c concentration in freshwater. In turn, ZUU, ZRU, ZUS and ZUR are mass flows of contaminants between units, regeneration to units, units to disposal and units to regeneration units. Finally $\Delta M_{u,c}$ is the mass load of component c.

Maximum inlet concentration at the water-using units

$$\begin{aligned}\sum_{w} \left(CW_{w,c} * FUW_{w,u}\right) + \sum_{u^*} ZUU_{u^*,u,c} + \sum_{r} ZRU_{r,u,c} \\ \leq \text{Cinmax}_{u,c} * \left(\sum_{w} FUW_{w,u} + \sum_{u^*} FUU_{u^*,u} + \sum_{r} FRU_{r,u} \right) \qquad \forall u, c\end{aligned} \tag{4}$$

Maximum outlet concentration at the water-using units

$$\begin{aligned}\sum_{w} \left(CW_{w,c} * FUW_{w,u}\right) + \sum_{u^*} ZUU_{u^*,u,c} + \sum_{r} ZRU_{r,u,c} + \Delta M_{u,c} \\ \leq \text{Coutmax}_{u,c} * \left(\sum_{u^*} FUU_{u,u^*} + \sum_{r} FUR_{u,r} + \sum_{u^*} FUU_{u,u^*} + \sum_{s} FUS_{u,s} \right) \quad \forall u, c\end{aligned} \tag{5}$$

Cinmax and *Coutmax* are maximum inlet and outlet concentrations.

Contaminant balance at the regeneration processes

$$\begin{aligned}ZR_{r,c}^{out} = \left[\sum_{u} ZUR_{u,r,c} + \sum_{r^*} ZRR_{r^*,r,c} \right] * (1 - XCR_{r,c}) \\ + \left[\sum_{u} ZRU_{r,u,c} + \sum_{r^*} ZRR_{r,r^*,c} + \sum_{r^*} ZRR_{r,r^*,c} \right] * XCR_{r,c} \qquad \forall r, c\end{aligned} \tag{6}$$

Here $XCR_{r,c}$ is a binary parameter that determines is a contaminant is removed or not.

Capacity (*CAP*) of the regeneration processes

$$CAP_r = \sum_{u} FUR_{u,r} + \sum_{r^*} FRR_{r^*,r} \quad \forall r \tag{7}$$

Contaminant mass loads

These constraints are written in a general form where i can be any water using unit or any regeneration process; and j can be a water using unit, regeneration process or sink.

$$ZIJ_{i,j,c} = FIJ_{i,j} * Cout_{i,j} \qquad \forall i \in \{U, R\}, j \in \{U, R, S\}, c \tag{8}$$

Freshwater consumption – Objective function

$$Min \sum_{w} \sum_{u} FWU_{w,u} \qquad (9)$$

3. The Discrete Methodology

3.1. Model Discretization

The proposed approach discretizes one variable (concentrations used here or flowrates) of the bilinear term generated at the splitting points. As a result, a mixed integer linear programming (MILP) model is generated. The discretized concentrations are now parameters ($DC_{d,c,u}$ for the water using units; $DCR_{d,c,r}$ for regeneration processes). Eq. 8 (the only bilinear one) is substituted by the following "big M" constraints, that force the outlet concentrations to be in between two discrete concentrations.

$$ZIJ_{i,j,c} - DC_{d,c,i} * FIJ_{i,j} \geq DC_{d,c,i} * \mathrm{Fmax} * \left(\mathrm{XI}_{\mathrm{i,c,d}} - 1\right) \qquad \forall i \in \{U,R\},\ j \in \{U,R,S\}, c, d < \mathrm{dmax} \qquad (10)$$

$$ZIJ_{i,j,c} - DC_{d+1,c,i} * FIJ_{i,j} \leq DC_{\mathrm{dmax},c,i} * \mathrm{Fmax} * \left(1 - \mathrm{XI}_{\mathrm{i,c,d}}\right) \qquad \forall i \in \{U,R\},\ j \in \{U,R,S\}, c, d < \mathrm{dmax} \qquad (11)$$

To guarantee that only one interval is picked, we write:

$$\sum_{d} \mathrm{XI}_{\mathrm{i,c,d}} = 1 \qquad \forall i \in \{U,R\}, c \qquad (12)$$

Thus, the contaminant mass load of each stream is calculated through a relaxation between two discrete points. Finally, to ensure that there is no contaminant mass load when flowrate does not exist, we write:

$$ZIJ_{i,j,c} \leq DC_{\mathrm{dmax},c,i} * \mathrm{FIJ}_{\mathrm{i,j}} \qquad \forall i \in \{U,R\},\ j \in \{U,R,S\}, c \qquad (13)$$

The discretized model provides a lower bound (because it is relaxing one constraint), but most important, it also points to a set of intervals that might contain the optimum. In addition, a good upper bound can be obtained using the solution of this lower bound as a starting point of the original NLP problem.

Once a lower bound and an upper bound of the problem are found, one can evaluate the lower bound solution and determine which intervals might be part of an optimum solution. The ones that are proved not to be in the optimum solution are eliminated and the remained intervals of the discrete concentration parameters are discretized again. This is done as follows.

3.2. Interval Eliminations

In each iteration, after a lower and an upper bound are found, we implement the following procedure for each discrete concentration:

1. The interval selected by the lower bound model is forbidden to be selected (this means the correspondent binary is fixed to zero)
2. The discrete model is then run again. Two possibilities exist:

a. The solution is feasible (a solution between the current lower and upper bound exists). In this case, it is possible to have an optimum solution outside of the investigated interval. Thus, nothing is done.
b. The solution is infeasible (there is no feasible solution between the current lower and upper bound outside of the investigated interval). Thus, the optimum solution needs is inside of the investigated interval. Thus, the region outside of the investigated interval is disregarded.

4. Illustration of The Methodology

We now illustrate the method a small example with two water-using units and two contaminants (Wang and Smith, 1994) (Table 1). For this example, two intervals (*dmax*=3) are used. Figure 1 shows how the discrete concentrations are being divided at the beginning (initialization step).

Table 1 – Limiting data of illustrative example

Process	Contaminant	Mass Load (Kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	4	0	100
	B	2	25	75
2	A	5.6	80	240
	B	2.1	30	90

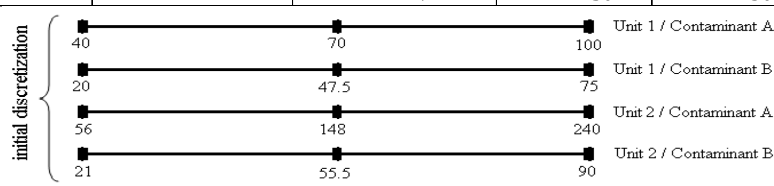

Figure 1 – Illustrative example of the discrete approach - initialization.

In this case, the lower bound is 52.895 ton/h and the upper bound is 54 ton/h. All the selected intervals of the discrete concentration are in the second interval. When the lower bound model is re-run forbidding the selected intervals (intervals evaluation), it is found that none of the first intervals have the possibility of hosting the optimum solutions. Thus, the intervals between the first and second discrete points can be eliminated and the second intervals re-discretized.

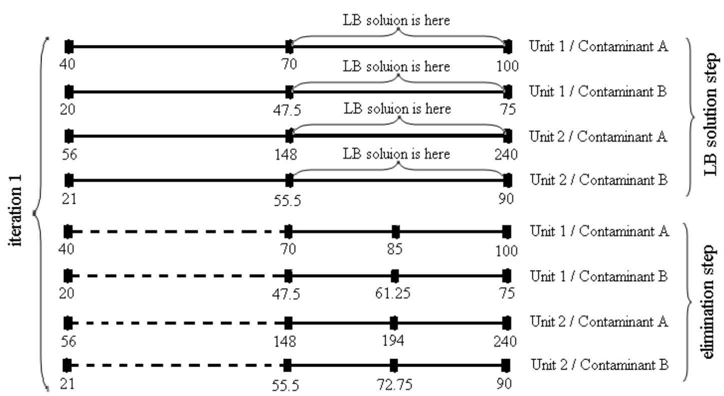

Figure 2 – Illustrative example of the discrete approach – 1st iteration.

With this new intervals in the second iteration the lower and upper bound do not change (LB = 52.895 ton/h and UB = 54 ton/h), but the intervals are smaller, so a new elimination procedure can be conducted. The same procedure is repeated until the lower bound solution is equal (or has a tolerance difference) to the upper bound solution. In this example, using two intervals, is solved in 11 iterations and 11.6 seconds. Note that hen the elimination is not possible more intervals are used.

5. Examples

The proposed method is applied to a refinery case presented by Koppol et al. (2003). This example has four key contaminants (salts, H2S, Organics and ammonia), six water using units, and three regeneration processes. The limiting data of the water using units are shown in the original paper. The solution when freshawater consumption is minimized, without allowing the addition of regeneration processes, is presented in Figure 3. A freshwater consumption of 119.332 ton/h was achieved. Only one iteration is needed and the solution is found in 0.81 seconds. The solution when regeneration processes are introduced (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 H_2S to 5 ppm and ammonia to 30 ppm) has a freshwater consumption of 33.571 ton/h. Only one iteration is needed to find the solution in 2 seconds. However, the found solution present several regeneration recycles and very small flowrates. This is an undesirable situation for the practical point of view. To overcome this issue, we added binary variables to control a minimum allowed flowrate if the connection exits and to forbid recycles as well. The new solution (also 33.517 ton/h) is found in two iterations (34 seconds). The flowsheet obtained is not shown for space reasons.

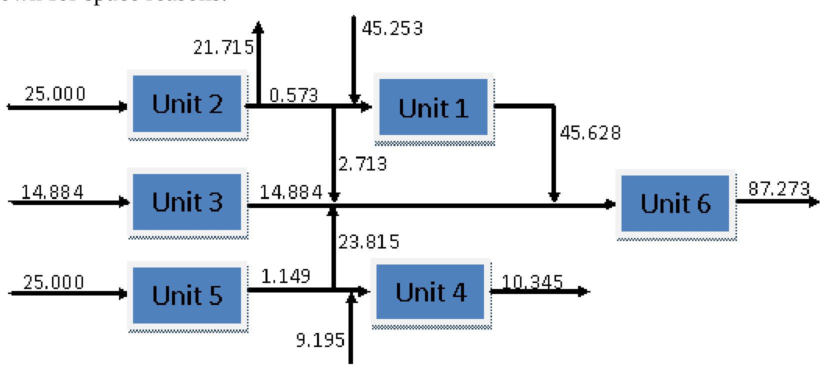

Figure 3– Optimum for Multicomponent Example. No regeneration

Further, we no longer consider the regeneration processes with fixed outlet concentrations of the key contaminants. Instead, we evaluate what would be these concentrations if we want minimize the need for regenerations at the found freshwater consumption (33.571 ton/h). To translate this goal to a mathematical form, we use the total removed contaminant mass load (that is the combination between flowrate and concentration reduction) as the objective function. Now, the outlet concentrations of the keys contaminants in the regeneration processes can have any value higher than the ones previously presented. The optimum solution found after 2 iterations (66 Seconds) shows the regeneration processes having the following features: Reverse osmosis needs to reduce salts to 85 ppm instead 20 ppm originally proposed. The API separator followed by ACA need to reduce organics to 50 ppm as before. Finaly, the Chevron wastewater treatment should keep the 5 ppm reductions for H_2S, but can operate to reduce ammonia to 120 ppm instead 30ppm. The suggested network is presented in Figure 4.

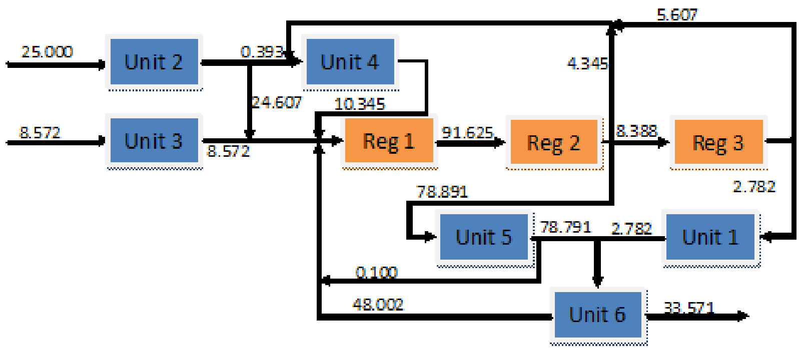

Figure 4– Optimum for Multicomponent Example. With Regeneration

6. Conclusions

The suggested approach has showed good results on the minimum water allocation problems. The methodology also allows handling the outlet concentration of the key contaminants of the regeneration processes as a variable. This arises to be important when one wants to determine optimum contaminats reduction without define the regeneration processes beforehand. As future work, the methodology will be extended to the optimization of WAP using other objective function.

References

M. Bagajewicz, 2000, A review of recent design procedures for water networks in refineries and process plants, Computers and Chemical Engineering, 24, 2093-2113.

M. Bagajewicz, M. Rivas and M. Savelski, 2000, A robust method to obtain optimal and sub-optimal design and retrofit solutions of water utilization systems with multiple contaminants in process plants, Computers and Chemical Engineering, 24, 1461-1466.

A.A. Alva-Argaez, C. Kokossis and R. Smith, 1998, Wastewater minimization of industrial system using an integrated approach, Computers and Chemical Engineering, 22, S741-S744.

A.A. Alva-Argaez, C. Kokossis and R. Smith, 2007, A conceptual decomposition of MINLP models for the design of water-using systems, Int. J. of Env. and Pollution, 29(1-3), 177-205.

C. Ullmer, N. Kunde, A. Lassahn, G. Gruhn and K. Schulz, 2005, WADO: water design optimization – methodology and software for the systhesis of process water systems, Journal of Cleaner Production, 13, 485-494.

R.Karuppiah and I.E. Grassmann, 2006, Global optimization for the systhesis of integrated water systems in chemical processes, Computers and Chemical Engineering, 30,650-673.

Y.P. Wang and R. Smith, 1994, Wastewater Minimization, Chem. Eng. Science, 49(7), 981-1006.

A.P.R. Koppol, M.J. Bagajewicz, B.J. Dericks and M.J. Savelski, 2003, On zero water discharge solutions in the process industry, Advances in Environmental Research, 8, 151-171.