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A New Heuristic Procedure for the Optimal Design of Wastewater Treatment Systems

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This paper outlines a new efficient solution strategy for the optimal design of wastewater treatment networks (WTN) with multiple contaminants. It consists of a two stage method aimed at finding global optimal solutions to the problem. In the first stage, the full problem is divided and each treatment unit is tackled one at a time. The general non-convex nonlinear program (NLP) is thus replaced by a sequence of related linear programs (LPs) and a feasible network is generated. Multiple NLPs are solved in the second stage, one for each sequence, and the best found solution is chosen as the optimal one. The results have shown that the proposed algorithm is more effective in escaping local optimal solutions than another approach taken from the literature.

1. Introduction

Several industrial processes require substantial amounts of water for their daily operation. These processes originate wastewater with a few contaminants, which may pose an environmental pollution problem. The traditional way of addressing this problem has always been on finding end-of-pipe solutions as the sole reply to the imposed discharge constraints. However, scarcity of water and strict regulations on industrial effluents have created new attitudes over water usage. The possibility of selectively reusing water and/or recycling it has become an option worth exploring, since it has a direct impact both on total water consumption in water using networks (WUN) and on wastewater generation heading for centralized or distributed treatment.

Since the seminal paper of Takama et al. (1980), who addressed the simultaneous optimization problem of both water using and treatment networks (WUTN) in a petroleum refinery with a NLP, many contributions have appeared. Recent ones can be found in Gunaratnam et al. (2005) and Karuppiah & Grossmann (2006). Most of the research, however, has focused on either the WUN or WTN problems, which are already challenging for multicontaminant systems. While modeling the problem as a non-convex NLP or mixed integer nonlinear program (MINLP) is straightforward, its solution is not. Global optimization algorithms like BARON or the one in Karuppiah & Grossmann (2006) are convenient but may require too much computational time for large problems. As an alternative, methods relying on faster local optimization solvers and multiple starting points can be employed. Teles et al. (2007) have proposed an efficient initialization procedure for the optimal design of WUN, where the general NLP is replaced by a succession of LPs each considering a single operation unit. While this work applies the same ideas to the WTN, the implementation has been more complex due to the fact that the treatment units are no longer independent, i.e. we have to ensure that the effluents leaving the system, when mixed, meet regulations.

2. Problem statement

This work addresses the optimal design of wastewater treatment systems. Given a number of wastewater streams (set W), containing well-defined pollutants (set C), with known concentrations ($c_{w,c}^{WWat}$), the target is to find the network configuration that minimizes the total flowrate of wastewater to be treated on a distributed treatment system featuring a predefined set of treatment units (set T), in order to reduce the concentration of the associated environmental pollutants (c_c^{Med}) down to the imposed limits at discharge point. The total flow of the various kinds of wastewater (tf_w^{WWat}), the removal ratios of each treatment process ($rr_{t,c}$), as well as the maximum inlet concentrations for every contaminant ($c_{t,c}^{In\,Max}$) are parameters assumed to be known.

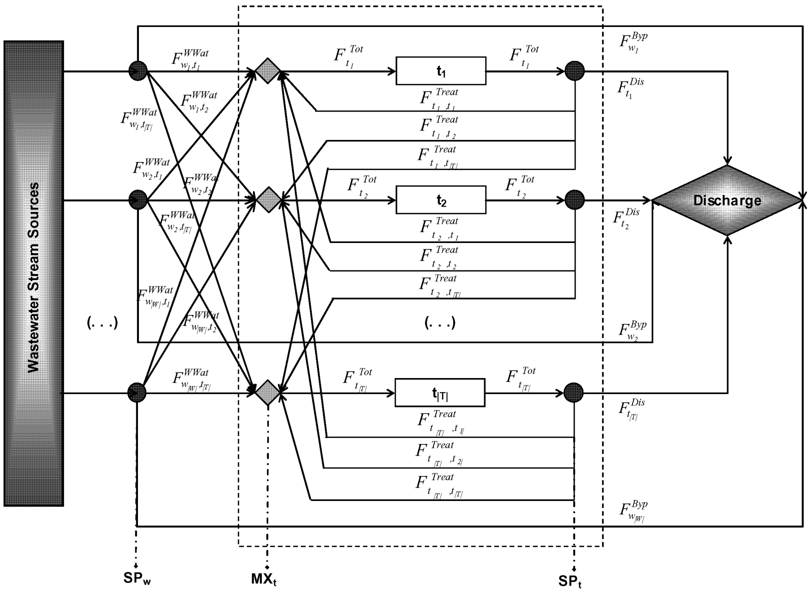

Figure 1. Superstructure of the wastewater treatment system design problem.

3. General NLP mathematical formulation

Similarly to other optimization studies on industrial water processing, a superstructure that entails all possible flow configurations is established as the foundation for the mathematical formulation. It includes the full set of wastewater streams and treatment units, as well as several nodes that are either stream splitters, located immediately after the original wastewater streams (SP_w) or after the treatment units (SP_t), or stream mixers (see figure 1). The latter can be either inlet mixers to the treatment units (MX_t) or the final discharge mixer located downstream that collects wastewater bypassing the treatment system together with treated effluents.

The mathematical model of the problem comprises the following variables: $F_{w,t}^{WWat}$ and F_t^{Tot}, flowrate of wastewater w and the total flowrate entering treatment t, respectively; $F_{j,t}^{Treat}$, total flowrate from treatment j to treatment t; F_w^{Byp} flowrate of wastewater w bypassing the treatment system and directly going to discharge point; F_t^{Dis} total flowrate from treatment t heading for the discharge point; and finally, $C_{t,c}^{In}$ and $C_{t,c}^{Out}$, the treatment units inlet and outlet concentrations, respectively.

The constraints for the general NLP are presented next. Eq 1 is the objective function which minimizes the total flow going into the treatment units. Eq 2 is the flow balance over the SP_w splitters. Eqs 3-4 are the total flow balance over the MX_t mixers and SP_t splitters. Eq 5 is the total mass balance over the MX_t mixers, where the inputs to treatment i come from both the original wastewater streams and from the same (recycling) or other treatment units' outlet streams. Eq 6 ensures that the concentration of the discharge stream does not exceed the maximum environmental limits. Eq 7 ensures that the inlet concentration to treatment t does not violate the maximum pre-defined limits for contaminant c. Eq 8 defines the removal ratio and eq 9 represents the upper bound on the inlet treatment concentrations.

$$Min \sum_{t \in T} F_t^{Tot} \tag{1}$$

$$tf_w^{WWat} = \sum_{t \in T} F_{w,t}^{WWat} + F_w^{Byp}, \quad \forall w \in W \tag{2}$$

$$F_t^{Tot} = \sum_{w \in W} F_{w,t}^{WWat} + \sum_{j \in T} F_{j,t}^{Treat}, \quad \forall t \in T \tag{3}$$

$$F_t^{Tot} = F_t^{Dis} + \sum_{t \in T} F_{t,j}^{Treat}, \quad \forall t \in T \tag{4}$$

$$F_t^{Tot} \cdot C_{t,c}^{In} = \sum_{w \in W} F_{w,t}^{WWat} \cdot c_{w,c}^{WWat} + \sum_{j \in T} F_{j,t}^{Treat} \cdot C_{j,c}^{Out}, \quad \forall t \in T, \forall c \in C \tag{5}$$

$$\sum_{w \in W} F_w^{Byp} \cdot c_{w,c}^{WWat} + \sum_{t \in T} F_t^{Dis} \cdot C_{t,c}^{Out} \le \sum_{w \in W} tf_w^{WWat} \cdot c_c^{Med}, \quad \forall c \in C \tag{6}$$

$$\sum_{w \in W} F_{w,t}^{WWat} \cdot c_{w,c}^{WWat} + \sum_{j \in T} F_{j,t}^{Treat} \cdot C_{j,c}^{Out} \le \left(\sum_{w \in W} F_{w,t}^{WWat} + \sum_{j \in T} F_{j,t}^{Treat} \right) \cdot c_{t,c}^{In\,Max}, \forall t \in T, \forall c \in C \tag{7}$$

$$C_{t,c}^{Out} = C_{t,c}^{In} \cdot \left(1 - rr_{t,c}\right), \quad \forall t \in T, \forall c \in C \tag{8}$$

$$C_{t,c}^{In} \le c_{t,c}^{In\,Max}, \quad \forall t \in AcT, \forall c \in C \tag{9}$$

4. Solution methods for NLPs

The above NLP includes non-convex equations arising from the presence of bilinear terms, which means that we may get stuck in a suboptimal solution if a local optimization solver is used. Typically, such solutions are strongly dependent on the starting point used, making the initialization procedure an important step of the overall solution method. If global optimization solvers are used, no such problem occurs but these are much more demanding computationally, which may prevent their practical use. Methods relying on the solution of a general NLP for multiple starting points can be thought of valid alternatives to global solution methods since in the limit of an infinite number of points they can find the global optimal solution.

For the design of wastewater treatment systems, Castro et al. (2007) have recently presented a two-stage effective heuristic procedure. The first part starts from a simplified superstructure that does not feature MX_t mixers, the source of nonlinear constraints. Since this option removes structures with units arranged in series, treatment systems comprising 2 to |T| units in series are added to the superstructure. The resulting LP can then be used to initialize the general NLP for a given sequence of treatment units. The second part of the algorithm merely solves the |T|! NLPs, differing only on the starting point used, and selects the best solution as the optimal one. When compared to the global optimization solver BARON in a collection of example problems, their method was always able to find the global optimal solution in considerable less time.

5. New initialization strategy

This paper proposes a new two-stage heuristic procedure for the optimal design of industrial wastewater treatment networks. It is named SIPOL (Serial Iterative Process Of Initialization) and differs from the method of Castro et al. (2007) in the initialization step. Now, the general NLP is split into |T| linear subproblems that are solved sequentially from the first to the last treatment in the sequence. For the active treatment unit, the problem is reduced to a LP simply because its possible inlet streams are either wastewater or treated outlet streams from all previous treatments (in the active sequence). While the inlet flowrates to the active unit still remain as model variables, all possible inlet streams have known concentrations (model parameters or values from previous iterations) and hence bilinear terms are avoided. The second stage involves the solution of the general NLP for all possible sequences of treatment units so, overall, the procedure involves the solution of |T|·|T|! LPs followed by |T|! NLPs. The best solution is assumed to be the global optimum, although there is no theoretical guarantee.

The LP formulation for active unit *t* and sequence *s* is presented next. It requires the definition of new sets and variables. $\wp_{s,t}$ is the set of all treatment units for which the position in sequence *s* is equal or greater than the one of unit *t* while $\Im_{s,t}$ is the opposite set. $M_{t,j,c}^{Treat}$ and $M_{j,c}^{Dis}$ represent the predicted mass concentrations from treatment *t* to treatment *j* or to the discharge point, respectively, for the actual and succeeding iterations. The parameters $f_{j,t}^{Treat}$, $f_{w,t}^{WWat}$, f_t^{Tot} and $c_{j,c}^{out}$ are known from previous stages. The objective function is eq 1 restricted to the active treatment unit. Eqs 10-11 are the flow balances over MX_j and SP_w. Eq 12 states that the flowrate from unit $j \in \wp_{s,t}$ does not exceed the flowrate into unit *j* (f_j^{Tot}) determined from previous iterations. Eqs 13-14 define feasibility constraints for every contaminant over the remaining problem (for units located in the sequence after treatment unit *t*) and ensure that the maximum environmental discharge limits are met.

$$F_j^{Tot} = \sum_{w \in W} F_{w,j}^{WWat} + \sum_{u \in \Im_{s,j}} F_{u,j}^{Treat}, \quad \forall s \in AcS, \forall t \in AcT, \forall j \in \wp_{s,t} \tag{10}$$

$$tf_w^{WWat} = F_w^{Byp} + \sum_{j \in \Im_{s,t}} f_{w,j}^{WWat} + \sum_{j \in \wp_{s,t}} F_{w,j}^{WWat}, \quad \forall s \in AcS, \forall t \in AcT, \forall w \in W \tag{11}$$

$$f_j^{Tot} \geq \sum_{u \in \wp_{s,j} \cap \Im_{s,t}} f_{j,u}^{Treat} + \sum_{u \in \wp_{s,t}} F_{j,u}^{Treat}, \quad \forall s \in AcS, \forall t \in AcT, \forall j \in \Im_{s,t} \tag{12}$$

$$\begin{aligned} &\left(\sum_{w \in W} \mathrm{F}_{\mathrm{w,j}}^{\mathrm{WWat}} \cdot \mathrm{c}_{\mathrm{w,c}}^{\mathrm{WWat}} + \sum_{u \in \Im_{\mathrm{s,t}}} \mathrm{F}_{\mathrm{u,j}}^{\mathrm{Treat}} \cdot \mathrm{c}_{\mathrm{u,c}}^{\mathrm{Out}} + \sum_{u \in \wp_{\mathrm{s,t}} \cap \Im_{s,j}} M_{u,j,c}^{Treat} \right) \cdot \left(1 - rr_{j,c}\right) \\ &= \sum_{\substack{u \in \wp_{\mathrm{s,j}} \\ u \neq j}} M_{j,u,c}^{Treat} + M_{j,c}^{Dis}, \forall s \in AcS, \forall t \in AcT, \forall j \in \wp_{\mathrm{s,t}}, \forall c \in C \end{aligned} \tag{13}$$

$$\begin{aligned} &\sum_{j \in \wp_{\mathrm{s,t}}} M_{j,c}^{Dis} + \sum_{j \in \Im_{\mathrm{s,t}}} \left(f_j^{Tot} - \sum_{u \in \wp_{\mathrm{s,j}} \cap \Im_{\mathrm{s,t}}} \mathrm{f}_{\mathrm{j,u}}^{\mathrm{Treat}} - \sum_{u \in \wp_{\mathrm{s,t}}} \mathrm{F}_{\mathrm{j,u}}^{\mathrm{Treat}} \right) \cdot \mathrm{c}_{\mathrm{j,c}}^{\mathrm{Out}} + \sum_{w \in W} \mathrm{F}_{\mathrm{w}}^{\mathrm{Byp}} \cdot \mathrm{c}_{\mathrm{w,c}}^{\mathrm{WWat}} \\ &\leq \sum_{w \in W} \mathrm{tf}_{\mathrm{w}}^{\mathrm{WWat}} \cdot \mathrm{c}_{\mathrm{c}}^{\mathrm{Med}}, \forall s \in AcS, \forall t \in AcT, \forall c \in C \end{aligned} \tag{14}$$

6. Example problem

A particular illustrate example from Castro et al. (2007) is given in table 1, featuring |W|=3, |C|=6 and |T|=5. SIPOL involved the solution of 720 problems, 5·5!=600 LPs + 120 NLPs and a total computational effort of 164 CPUs. The best solution found is characterized by a total treatment flow of 124.359 t/h, with two wastewater streams bypassing the treatment system directly to the discharge point, one partially, see figure 2. It is important to mention that SIPOL generates feasible water networks and that 8 of the 120 initialization points led to the optimal solution. The method of Castro et al. (2007) starts from networks that are somewhat infeasible but that pose no convergence problems for the local optimization solvers. For this example, their best solution was slightly inferior to ours, 124.442t/h, but was found in significantly less time (14 CPUs), due to the solution of a lower number of problems (120 LPs+120 NLPs). BARON reached the exact same solution but could not prove global optimality in 1 h.

For the other 8 examples in Castro et al. (2007), SIPOL was able to reach the global optimal solution and in half of them, the initialization procedure itself (for at least one of the sequences) was able to find the optimum. The computational effort was typically one order of magnitude larger than for Castro et al. (2007) but was substantially lower to that of BARON.

7. Conclusions

This paper has presented a new LP-based initialization strategy for the optimal design of wastewater treatment networks with multiple contaminants through the solution of a NLP. It generates multiple feasible starting points, one for every possible sequence of treatments, and assumes that the best solution found is the global optimal solution. The new strategy was shown to be more effective in avoiding local optimal solutions than the method of Castro et al. (2007), as illustrated through the solution of a complex example problem taken from the literature. Future work will include the generalization of the method for other objective functions (e.g. that include capital cost terms) and for other performance measures of the treatment units (e.g. fixed outlet concentrations instead of fixed removal ratios).

Table 1. Problem data for example problem

	$c_{w,c}^{WWat}$					$rr_{t,c}$					
Contaminant (c)	w1	w2	w3	w4	w5	t1	t2	t3	t4	t5	c_c^{Med}
A	1100	40	200	60	400	0.99					100
B	500	-	220	510	170		0.99				100
C	500	100	200	500	100			0.99			100
D	200	300	500	200	300				0.99		100
E	800	910	150	780	900				0.90	0.99	100
F	100	200	-	100	-					0.99	100
tf_w^{WWat}	19	7	8	6	17						

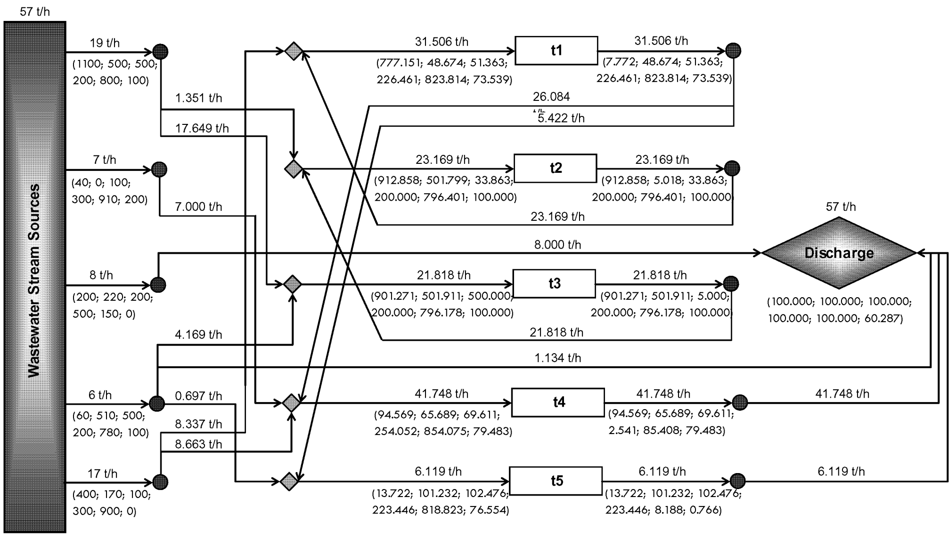

Figure 2. Optimal wastewater treatment network for example problem.

8. References

Castro, P., H. Matos and A. Novais, 2007, Resources Conservation Recycling, 50, 158.

Gunaratnam, M. et al., 2005, Ind. Eng. Chem. Res., 44, 588.

Karuppiah, R. and I. Grossmann, 2006, Comp. Chem. Eng., 30, 650.

Takama, N., Kuriyama, T., Shiroko, K., Umeda, T., 1980, Comp. Chem. Eng., 4, 251.

Teles, J. et al., 2007, LP-based Solution Strategies for the Optimal Design of Industrial Water Networks with Multiple Contaminants, Submitted to Chem. Eng. Sci.