CHEMICAL ENGINEERING TRANSACTIONS Volume 18, 2009
Editor Jiří Klemeš

DOI: 10.3303/CET0918023

Optimal Design of Wastewater Treatment System through a MILP-based Initialization Procedure

João Teles[1,2], Pedro Castro*, Henrique A. Matos[2]
[1]Dep. de Modelação e Simulação de Processos, INETI, 1649-038, Lisboa, Portugal
[2]Dep. Engenharia Química e Biológica, IST, 1049-001, Lisboa, Portugal
pedro.castro@ineti.pt

This work presents a new approach for the optimal design of distributed wastewater treatment networks (WTN) featuring multiple contaminants. It consists of a two-stage solution procedure. The first stage makes use of a sequence of mixed-integer linear programs (MILP) to generate a striking number of structurally different suboptimal networks. Each will correspond to a starting point for the solution of the general non-linear program (NLP), in the second stage. The initialization strategy assumes that the wastewater streams go through the treatment units in series from the moment they enter the system up to the discharge point. On each calculation stage, binary variables are used to select the best unit for that position, while ensuring that the remaining treatment units are powerful enough to take the contaminants concentration down to the discharge limits. The approach is illustrated through the solution of several test cases taken from the literature and compared to that of our previous algorithm. Best solution returned and total computational efforts are the critical indicators for model performance evaluation.

1. Introduction

Most industrial processes require substantial amounts of water for their daily operation. They also generate contaminated wastewater streams that must be treated down to the pollutants environmental discharge limits before being released to the environment. Traditionally, wastewater streams from different process operations have been mixed and sent to centralized treatment systems in order to meet discharge regulations. However, lower operating costs can be achieved with a distributed treatment system, where different wastewater streams go to different treatment units.
In this paper, it is assumed that we are given a set of wastewater streams characterized by flowrate and concentration, treatment units with fixed removal ratios, and maximum discharge limits for every contaminant. The objective is to minimize the total inlet flowrate to the treatment units. The problem can be formulated as a nonlinear program (NLP) but due to the presence of non-convex bilinear terms, it may be difficult to find global optimal solutions through the use of local optimization solvers. One can use global optimization solvers or algorithms specifically suited to the integrated water-using/treatment (WUTN) design problem, like the one proposed by Karuppiah and Grossmann (2006), that guarantee global optimality but may require a substantially, if

Please cite this article as: Teles J., Castro P. and Matos H., (2009), Optimal design of wastewater treatment systems through a milp-based initialization procedure, Chemical Engineering Transactions, 18, 153-158 DOI: 10.3303/CET0918023

not prohibitive, amount of computational resources. A trade-off can be achieved with heuristic procedures such as solving the general NLP several times starting from structurally different initial points. Examples of such methods, that are very effective at finding the global optimal solution, can be found in our recent work (Castro et al., 2007, 2009). However, they are not entirely efficient, and are limited in practice to a system of seven treatment units.

The proposed initialization procedure also assumes that the wastewater streams go through the treatment units in sequence from the moment they enter the system up to the discharge point. However, instead of fixing a unit to a certain position in the sequence and considering all possibilities, there is now a binary decision variable that chooses the best operation for a certain position. On the whole, one MILP is required per unit. The new procedure is fairly fast but is also not totally efficient in finding the global optimum due to its inherent singularity. To overcome this drawback, one can specify the first operation in the sequence, and consequently generate multiple starting points for the NLP. Such MILP-based procedure has been successfully applied to the design of water-reuse units (Teles et al., 2009), without compromising the finding of the global optimal solution.

In this paper, the approach of Teles et al., 2009, is extended to the design of WTNs, which is considerably more challenging since in each calculation stage it has to be ensured that the remaining treatment units are powerful enough to take the contaminants concentration down to the discharge limits. The performance of the new method is illustrated through the solution of test cases taken from the literature and compared to that of our previous algorithm and also to the one embedded in the global optimization solver BARON.

2. Problem statement

Given a set *S* of process wastewater streams containing well-defined pollutants (set *C*), that must be partially removed, with known flowrates f_s^{ww} and concentrations $c_{s,c}^{ww}$. A set *T* of treatment units (*t*) are available and are characterized by maximum inlet concentrations $c_{t,c}^{in\,max}$ and fixed removal ratios $rr_{t,c}$. The objective is to minimize the total flowrate going through the treatment units while keeping the concentration of all contaminants in the process outlet effluent stream below discharge regulations c_c^{env} .

3. General Superstructure

Castro et al. (2007) have highlighted that there are two model alternatives, depending on the type of variables, chosen to model the WTN design problem. One uses total flows and component concentrations as model variables; the other, relies on total flows, component mass flows and split fractions. In this work, we use the former alternative. The corresponding formulation is well-known and can be seen for example in Castro et al., (2007). Strategically, to find the optimal WTN we must first account for all possible ways of treating the system's inlet wastewater streams. These are embedded in a general superstructure of the network, first proposed by Wang and Smith (1994). Such superstructure, given in Figure 1, includes the full set of wastewater streams and treatment processes as well as several other nodes that are either splitters (circles) or mixers (diamonds). The splitters are divided into two subsets: SP_s, located immediately after the original wastewater streams and SP_t located after the treatment units. In general, the optimal network structure will be rather complex featuring some treatment units in series and others in parallel and also stream recycle.

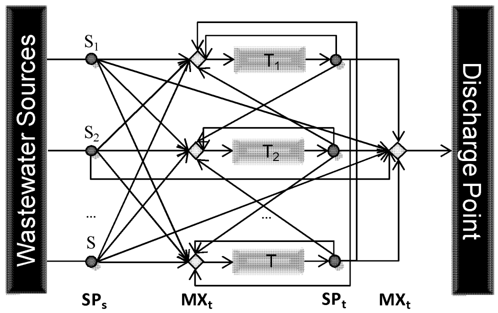

Figure 1. General superstructure for the wastewater distributed treatment system design problem (circles and diamonds indicate respectively, splitters, SP, and mixers, MX).

4. Proposed Method

The above NLP problem formulation gives arise to some bilinear terms, meaning that we may get trapped in a suboptimal solution if a local optimization solver is used. Methods relying on the solution of a general NLP for multiple starting points can be thought of valid alternatives to global solution methods with local solvers, since in the limit (a very large number of points) they can find the global optimal solution with, every so often, extremely less computational effort when compared to global solvers. However, the variables of the NLP need to be properly initialized to ensure a satisfactory optimal solution. Based on the above premise, Teles et al. (2009) have presented a strategy for the design of WUNs that serves now as source of inspiration for WTNs. Figure 2 displays the basic structure underneath the new initialization procedure (M1) for n streams an 3 treatment units.

To generate a good feasible solution to the problem, the optimizer starts by selecting, amongst all operations, the one that requires the lowest total wastewater intake for the first position in the sequence, through a single MILP. The binary variables (Y_t) are accountable to enable only a positive inlet of wastewater flow to the one for which the integer variable in stage 1 retrieves the value 1 (the dark unit in Figure 2). Identical procedure takes place in the second stage. Now the available wastewater sources are the remaining system's wastewater sources and also the cleaned outlet flow from the previously selected unit (set *PrT*), which can no longer take any more positions in the sequence. Thus, the solver is restricted to the selection of one of the remaining units (set *ReT*). The MILP phase of a particular sequence is finished when all units have been solved. Relatively to the example illustrated by Figure 2 which considers the final sequence T3-T1-T2, the following set elements were successively considered: for the first MILP, *ReT*={T1,T2,T3} and *PrT*={}; for the second MILP, *ReT*={T1,T2}, *PrT*={T3}, for the third MILP, *ReT*={T2} and *PrT*={T1,T3}. That serial network is then used as a starting point for the solution of the general NLP in an attempt to find an improved solution to the problem. Overall, to determine the optimal solution, this simple method requires the solution of #(*T*) MILPs followed by 1 NLP. In order to increase the probability of escaping local optima, the implemented algorithm considers that the first position in the sequence is fixed and generates #(*T*) starting points which are individually optimized to obtain a set of alternative networks. The best of the corresponding NLP solutions is then assumed to be the global optimal design, although there is not guarantee that it is so.

To model the initialization procedure we consider the lower case parameters ps_t, which give the position of unit *t* in the active sequence, and $f_{s,t}^{wt}$ to represent the flowrates of wastewater *s* into previous treatment units (that have been determined in preceding MILP blocks). The following variables are also considered: $F_{s,t}^{wt}$ represents the flowrate of wastewater *s* going into treatment unit *t*; F_s^{byp} gives, respectively, the flowrate of wastewater *s* that bypasses the treatment system directly do the final discharge and F_t^d the outlet flowrate from unit *t* to the same destination. F_t^t is the flowrate entering/leaving treatment unit *t*; $F_{t,t'}^{bt}$ represents the flowrate from treatment unit *t* to *t*'. The outlet mass flow of contaminant *c* from unit *t* is given by $M_{t,c}^t$, the discharge flow from unit *t* by $M_{t,c}^d$, and the mass flow from treatment unit *t* to unit *t*' by $M_{t,t',c}^{bt}$.

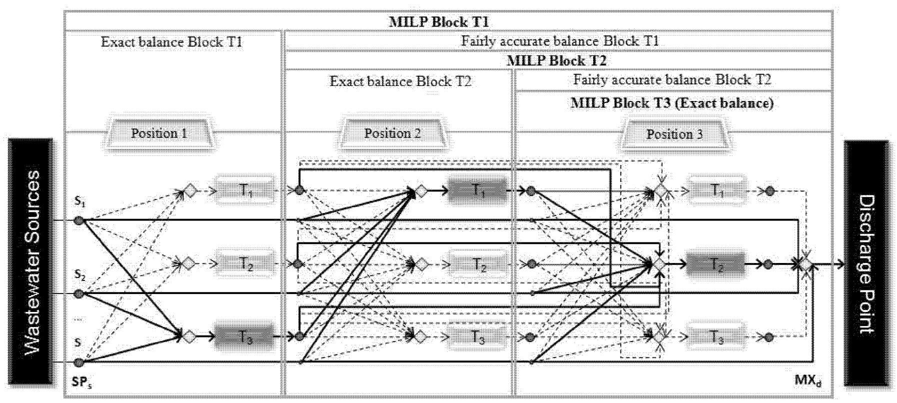

Figure 2. New general decomposition approach for the substructure corresponding to sequence T3-T1-T2. (Draft lines represent all possible initialization connections; continuous lines a particular generated sequence.)

The model constraints are given next: eq 1 defines the objective function, the minimization of the total flowrate going through the remaining treatment units. Eq 2 concerns the contaminant balances over the SP_s splitters. Eq 3 is the contaminant balance over the mixer of the active treatment unit. Eq 4 replaces the mass balance over the active unit's mixer and ensures that the maximum inlet concentrations are not exceeded. The flow balance is given in eq 5, where the flowrate into unit *t* (f_t^t) and those from t to previous units t' located after t in the sequence ($f^{bt}_{t,t'}$) have previously been determined. Eq 6 ensures that the remaining units are efficient enough to further decrease the contaminants load down to the environmental discharge limits. Eq 7 represents the mass balance over the remaining treatment units, where the outlet mass flow is related to the unit's inlet mass flow and removal ratio. Eq 8 is the mass balance over all SP_t splitters.

Notice that for previous units, the knowledge of the outlet concentrations enables us to know the exact contaminant mass flows for a particular unit from the related flowrate, eq 9. For the others, the best approach is to ensure that the discharge and outlet mass flows to succeeding units are set to zero if the corresponding flows are zero (eqs 10-11). This is the reason why the mass balances are only exact up to the splitter corresponding to the active unit (not including it).For the upper bounds we have used the maximum outlet concentrations. Eq 12 ensures a zero inlet flowrate for non-selected treatment units. The sum of total inlet wastewater to the system acts as the upper bound. Finally, to guarantee that a single unit is assigned to each calculation stage, eq 13 is used.

$$Min \sum_{t \in ReT} F^t_t \tag{1}$$

$$f^{ww}_s = F^{byp}_s + \sum_{t \in PrT} f^{wt}_{s,t} + \sum_{t \in ReT} F^{wt}_{s,t} \quad , \forall s \in S \tag{2}$$

$$F^t_t = \sum_{s \in S} F^{wt}_{s,t} + \sum_{t' \in PrT \wedge ps_{t'} < ps_t} F^{bt}_{t',t} \quad , \forall t \in ReT \tag{3}$$

$$\sum_{s \in S} F^{wt}_{s,t} c^{ww}_{s,c} + \sum_{t' \in T \wedge ps_{t'} < ps_t} M^{bt}_{t',t,c} \le F^t_t c^{inmax}_{t,c} \quad , \forall t \in ReT, c \in C \tag{4}$$

$$f^t_t \Big|_{t \in PrT} + F^t_t \Big|_{t \in ReT} = \sum_{t' \in PrT \wedge ps_{t'} > ps_t} f^{bt}_{t,t'} + \sum_{t' \in ReT \wedge ps_{t'} > ps_t} F^{bt}_{t,t'} + F^d_t \quad , \forall t \in T \tag{5}$$

$$\sum_{s \in S} F^{byp}_s c^{ww}_{s,c} + \sum_{t \in T} M^d_{t,c} \le f^{td} c^{env}_c \quad , \forall c \in C \tag{6}$$

$$M^t_{t,c} = \Big(\sum_{s \in S} F^{wt}_{s,t} c^{ww}_{s,c} + \sum_{t' \in T \wedge ps_{t'} < ps_t} M^{bt}_{t',t,c}\Big) \cdot (1 - rr_{t,c}) \quad , \forall t \in ReT, c \in C \tag{7}$$

$$f^t_t c^{out}_{t,c} \Big|_{t \in PrT} + M^t_{t,c} \Big|_{t \in ReT} = \sum_{t' \in PrT \wedge ps_{t'} > ps_t} f^{bt}_{t,t'} c^{out}_{t,c} + \sum_{t' \in ReT \wedge ps_{t'} > ps_t} M^{bt}_{t,t',c} + M^d_{t,c} \quad , \forall t \in T, c \in C \tag{8}$$

$$F^{bt}_{t,t'} c^{out}_{t,c} = M^{bt}_{t,t',c} \quad , \forall t \in PrT, t' \in ReT, c \in C \tag{9}$$

$$M^d_{t,c} \le F^d_t c^{inmax}_{t,c} (1 - rr_{t,c}) \quad , \forall t \in ReT, c \in C \tag{10}$$

$$M^{bt}_{t,t',c} \le F^{bt}_{t,t'} c^{inmax}_{t,c} (1 - rr_{t,c}) \quad , \forall t \in ReT, t' \in T, ps_{t'} > ps_t, c \in C \tag{11}$$

$$F^t_t = \sum_{s \in S} f^{ww}_s \, Y_t \quad , \forall t \in ReT \tag{12}$$

$$\sum_{t \in ReT} Y_t = 1 \tag{13}$$

5. Computational studies

Table 1 illustrates the performance of the new strategy through the solution of eight example problems taken from the literature (Castro et al., 2009). The computational study was performed in an Intel Core 2 Duo 2.4 GHz processor, with 2 GB of RAM memory, running Windows XP Professional. The algorithm and underlying mathematical formulations were implemented and executed in GAMS 22.5. The range of MILPs was treated with CPLEX, while the NLPs were solved by the local solver CONOPT and also by the global solver BARON. The results have shown that the best MILP solution is in some cases a near optimal solution. The novel strategy is further restrictive and hence slightly less effective when compared to model CTN (Castro et al., 2009). Since CTN scans over a higher number of structurally distinct initial points, it is somewhat natural that the chances to escape local optima are improved. Although, the new strategy proposed (M1) succeeds in terms of computational effort when compared to both CTN and BARON.

Table 1. Objective Function values (t/h) and total CPU effort (s)

	Best Initialization (t/h)		Best NLP (t/h)		BARON (t/h)	Total effort CPU (s)		
	CTN	M1	CTN	M1		CTN	M1	BARON
EX2	152.727		130.703			0.9	1.72	0.06
EX3	99.495		99.495			0.8	0.97	0.14
EX4	89.836		89.836			0.7	0.75	0.17
EX5	287.881		229.701	231.881	229.701	2.6	1.6	4.88
EX6	244.425		176.561		173.478	2.9	1.82	17
EX7	85.669		80.779	81.567	80.779	2.7	1.72	12.1
EX8	110.396		109.401			3.1	1.69	204
EX9	139.488	173.916	124.359	135.969	129.841[b]	140	9.89	3600

[b] Unable to prove global optimality (lower bound at time of interruption = 110.384).

6. Conclusions

This paper has extended the MILP-based method of Teles et al. (2009) for the optimal design of water treatment networks. It is a decomposition approach that divides the general network superstructure of the problem into multiple sequential substructures generated through dynamic sets. On each stage of the decomposition process, the solver selects a single unit to tackle through the solution of MILP that ensures that the downstream effluent meets environmental discharge limits. The performance of the new approach was tested with some example problems taken from the literature and was compared to our previous algorithm and to the global solver BARON. Overall, it is more efficient computationally for large problem sizes but is slightly less effective at finding the global optimal solution.

References

Castro P et al., 2007, Resources Conservation & Recycling 50, 158.

Castro P, Teles J, Novais A, 2009, Clean Technologies Environmental Policy 11, 83-93

Karuppiah R, Grossmann IE, 2006, Comput. Chem. Eng. 30, 650.

Teles J, Castro P, Novais A, 2009, MILP-based initialization strategies for the optimal design of water-using networks, Submitted to Chem. Eng. Sci.

Wang Y, Smith R, 1994, Chem. Eng. Sci 49, 3127.