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General Framework for Solving the Design and Operation of Wastewater Treatment Networks

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Abstract

This work addresses the design and operation of treatment systems for processing a set of wastewater streams in the most efficient way, thus solving the trade-off given by the minimization of investment, operational and environmental costs. An open framework is proposed for solving treatment networks, including any kind of objective function or treatment models. An evolutionary simulation-based search allows determining practical solutions to the design and operation problems. A case study including new aspects as energy balances and non-linear degradation rates is addressed for demonstrating the capabilities and flexibility of the approach and tool developed.

Keywords

Distributed Wastewater Treatment, Network Simulation, Stochastic Search.

1. Introduction

The problem of treatment networks consists of solving the trade-off between mixing and segregating effluents, the trade-off between large general treatment systems and multiple specific networked treatments. This problem requires modeling decisions on stream splitting and recycling leading to bilinear terms, multiple local optima and problems for standard solvers to converge. The

design problem is defined by different NLP and MINLP models for the design superstructure [1]. Global or near optimal solutions were shown to be attained in many cases by solving sequentially a relaxed linear model and the original MINLP [2] and rigorous global optimization was addressed via disjunctive programming [3]. Recently, a MINLP model included complex tradeoffs such as operating and capital costs, as well as piping and sewer costs [4]. Stochastic or meta-heuristic techniques have received less attention, though they easily manage solution feasibility, a drawback of the math programming approaches. Moreover, they are robust and admit any changes in the objective function as well as any kind of treatment model. Genetic algorithms [5] and guided random search of the feasible subspace [6] were used towards this end.
While the design problem requires more attention regarding the modeling detail, the network operation is hardly addressed. In this work, complex treatment models as well as component interaction (given by the effect of temperature) are included the design problem and for solving optimization of network operation under changing conditions. Problem formulation is presented and, finally, a software tool is presented implementing all this aspects in a open environment admitting the plug-in of any kind of treatment models or objective functions.

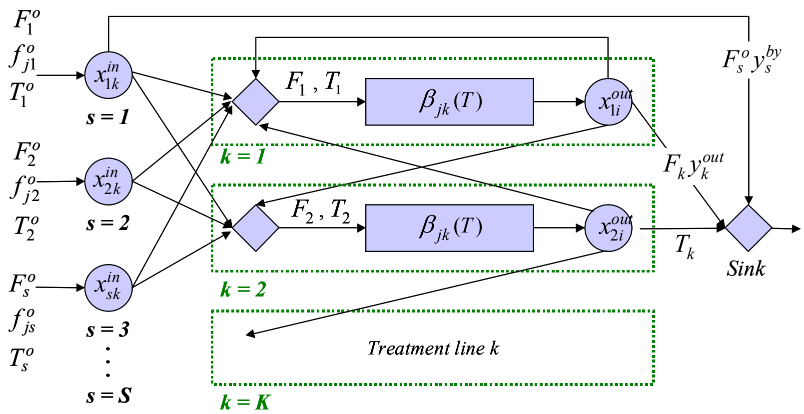

Figure 1: Problem superstructure defining problem variables and parameters

2. Problem Formulation

An extended problem formulation is derived from the problem superstructure given in figure 1, which also defines problem variables and parameters. The initial formulation [6] is adapted in order to include the energy balance, defined by the temperatures of the inlet streams T_k and their heat capacities CP_k. The split fractions determine the operating temperature at each treatment unit, which in turn changes of degradation rate β_{jk} of the contaminants. The operation of the system is given by the following constraints. First, mass balance in each splitter:

$$\sum_{k\le K} x_{sk}^{in} + y_s^{by} = 1 \quad \forall s, \quad 0 \le y_s^{by} \le 1 \ \forall s, \quad 0 \le x_{sk}^{in} \le 1 \quad \forall s,k \tag{1}$$

$$\sum_{i\le K} x_{ki}^{out} + y_k^{out} = 1 \quad \forall k, \quad 0 \le y_k^{out} \le 1 \ \forall ki, \quad 0 \le x_{ki}^{out} \le 1 \quad \forall ki \tag{2}$$

and total mass balance:

$$\sum_{k=1}^{K} F_k y_k^{out} + \sum_{s=1}^{S} F_s^o y_s^{by} = \sum_{s=1}^{S} F_s^o = F^T \tag{3}$$

The flows (total and for each contaminant) in each treatment line k are given by the fresh contribution plus the flows recycled from other treatment lines.

$$F_k = \sum_{s=1}^{S} F_s^o x_{sk}^{in} + \sum_{i=1}^{K} F_i x_{ik}^{out} \quad \forall k \tag{4}$$

$$f_{jk} = \sum_{s=1}^{S} f_{js}^o x_{sk}^{in} + \sum_{i=1}^{K} f_{ji}\left(1-\beta_{jk}\right) x_{ik}^{out} \quad \forall j,k \tag{5}$$

Accordingly, and assuming no phase change, the energy balance is given by:

$$F_k CP_k T_k = \sum_{s=1}^{S} F_s^o CP_s T_s x_{sk}^{in} + \sum_{i=1}^{K} F_i CP_i T_i \left(1-\Delta T_k\right) x_{ik}^{out} \quad \forall k \tag{6}$$

which, assuming also the same heat capacities and no temperature degradation *(ΔT_k)* due to heat losses or reaction heat, results in a weighted mean:

$$F_k T_k = \sum_{s=1}^{S} F_s^o T_s^o x_{sk}^{in} + \sum_{i=1}^{K} F_i T_i x_{ik}^{out} \quad \forall k \tag{7}$$

The recycle solving is achieved iteratively once the set of decision variables (x_{sk}^{in}, x_{ki}^{out}, y_s^{by}, y_k^{out}) is fixed and the treatment inlets (mixer outlets) are set as tear streams. Hence, for any general variable Z_k (and parameters λ_s and μ_k):

$$Z_k^{(n+1)} = \sum_{s=1}^{S} \lambda_s Z_s^o x_{sk}^{in} + \sum_{i=1}^{K} \mu_i Z_i^{(n)} x_{ik}^{out} \quad until \quad \left| Z_k^{(n+1)} - Z_k^{(n)} \right| \le \varepsilon_k \tag{8}$$

Yet, the convergence of the recycle calculation is only guaranteed if the set of decision variables corresponds to a feasible solution. This is part of the search procedure is explained in the next section. Finally, the optimization problem is set by establishing the objective function.

$$\min Z = f(F_k) \rightarrow \sum_{i=1}^{K} F_k \quad s.t. \quad \sum_{i=1}^{K} f_{jk}\left(1-\beta_{jk}\right) y_k^{out} \le C_j^{\max} F^T \quad \forall j \tag{9}$$

The design objective may depend on concentrations and flows in a complex way, but it is usually assumed to be the total flow processed, which is to be minimized. Unless operational issues are considered, the environmental aspects are usually regarded as constraints, thus a release limit for each pollutant results in the cheaper design polluting as much as allowed. When addressing the operation problem, the environmental issues are included in the economical cost objective to be minimized in the form of disposal charges. In this case, new constraints may appear because of the limitations given by the fixed treatment capacity. This will be described for the specific case study considered.

3. Search procedure and simulation

For the design problem, the set of feasible starting points is defined by the following constraints, which have to be met once given a treatment line k^*:

$$x_{sk^*}^{in} = 1 \qquad \forall s; \qquad \sum_{i=1}^{K} x_{ki}^{out} = 1 \qquad \forall k \neq k^* \tag{12}$$

$$x_{sk}^{in} = 0 \qquad \forall s, k \neq k^*; \qquad x_{s}^{by} = 0 \qquad \forall s; \quad x_{k^*i}^{out} = 0 \quad \forall i \tag{13}$$

This corresponds to a set of obvious and expensive cases consisting of mixing and processing all input streams serially through all treatment lines. For the operation problem, the best feasible starting point is the current solution in use.

Given a feasible starting point and a step-size *dx*, the feasible space is explored by a procedure [5] that randomly changes variable values x_p while keeping local and global balances. For each change, recycles are iteratively solved, the objective function evaluated, and the change accepted or not. The search is a greedy and fast downhill moving, but coupled with an exhaustive search of the current neighborhood to identify and escape local optima [5].

4. Software Design: modularity and customization

A software tool has been developed for solving and optimizing the treatment network attending the paradigms of flexibility, reusability and modularity and providing external configuration capabilities for incorporating custom treatment modules and allowing the tailoring of the objective function. The software class' constructor has the number of feeds, treatment units and number of contaminants (parameters) and creates dynamically all the structures to contain the data. This class has an optimization method implementing the search strategy. The objective function is implemented as a separate function included in a library providing user-friendly tools for managing this function. A separate function for the treatment allows a library of different treatment modules, from simple constant degradation rates to *ad-hoc* simulations of specific processes.
In addition, what-if analysis is provided via manual changes, as the input of feasible decisions for simulating and evaluating given a network configuration. Finally, the user interface allows controlling the search by means of diverse

pause/change/restart features and the display of the evolution of the objective function value as well as significant bounded variables (Fig. 2).

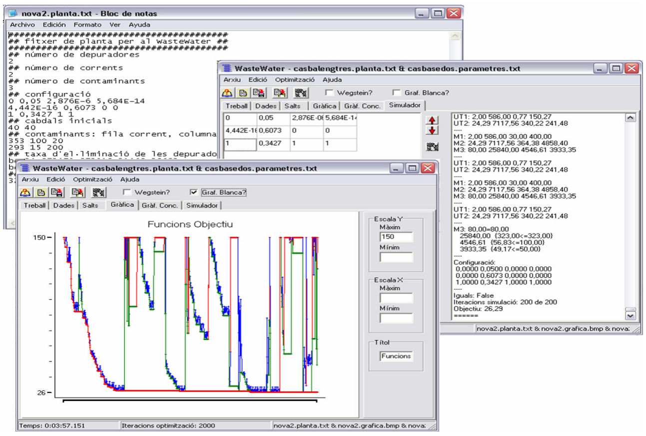

Figure 2: Software Interface

5. Case study

Two case studies are based on Example 1 [2], consisting of two inlet streams, two contaminants (A, B) and two treatment units. The input data is given in Table 1 (kinetic parameters) and Table 2 (Scenario 1): flow-rates, contaminant concentrations (ppm), and additional inlet temperatures. Assuming first-order kinetics and modeling treatment units as CSTR, degradation rates are given by:

$$df_{jk}\big/dt = -\kappa_{jk} f_{jk} \quad \Rightarrow \quad \beta_{jk} = 1-\left(1+\left(V_k \kappa_{jk}/F_k\right)\right)^{-1} \qquad \text{being} \quad \kappa_{jk} = A_{jk} e^{-E^a_{jk}/RT_k} \qquad (16)$$

which means that for the operation problem capacities for treatment units (V_k) have also to be included. The temperature effect on degradation rates may be significant in industrial cases such as the paper milling and illustrates how the approach developed addresses a non-linear issue such as component interaction. For the first scenario, the decision variables are the optimum values [2] for the original design problem (Table 2 – 1a). This is a feasible starting point for the operation problem set by a new objective Z defined as the sum of the outlet concentrations (ppm). For this new problem, solution 1a is improved by 20% (1b). The operation problem also means re-adjusting process variables when changes in market or supply conditions occur. In this case, this is given by a change on the inlet condition (scenario 2). This new state results in a 477% increase in the environmental cost (2a) that may be mitigated by the finding of a new solution reducing the cost by 53%. Certainly, changing temperatures also modifies degradation rates, thus the solution in scenario 2. Temperature adjustment (and associated costs) sets another problem with additional variables that poses a new challenge in formulating a new objective, but the solution approach presented would not be affected.

Table 1: Kinetic parameters.

A_{11}	A_{12}	A_{21}	A_{22}	Ea_{11}	Ea_{12}	Ea_{21}	Ea_{22}
873078	793683	872914	793611	31068	39061	872914	793611

Table 2: Problem data.

	F_1^0	T_1^0	ppm A	ppm B	F_2^0	T_2^0	ppm A	ppm B	V1	V2
Scenario 1	40	353	100	20	40	293	15	200	30	20
Scenario 2	20	353	10	120	50	293	150	20	30	20

Table 3: Solutions for the different problem scenarios.

	x_{11}^{in}	x_{22}^{in}	x_{12}^{out}	x_{21}^{out}	y_1^{out}	y_2^{out}	ppm A	ppm B	Z
1a	1.0000	1.0000	0.2750	0.0000	0.7250	1.0000	12.82	5.75	18.52
1b	1.0000	0.6800	0.9700	0.0000	0.0000	0.9975	10.00	5.85	15.85
2a	1.0000	0.6800	0.9700	0.0000	0.0000	0.9975	72.76	2.82	75.58
2b	1.0000	0.0000	0.9450	0.0000	0.0000	0.7538	32.54	3.40	35.94

6. Conclusions

Wastewater treatment networks have been addressed from the perspective of both, design and operation. A general problem formulation has been presented including new non-linear elements such as component interaction in the from of temperature and the consideration of energy balances and variable degradation rates. A robust stochastic search method has been used for solving the operation of the treatment network and results obtained show its viability and potential for addressing further problems such as the on line operation of the network.

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