NEOS Server Usage in Wastewater Treatment Cost Minimization

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Abstract. This paper describes the optimal design and operation of an activated sludge system in wastewater treatment plants. The optimization problem is represented as a smooth programming problem with linear and nonlinear equality and inequality constraints, in which the objective is to minimize the total cost required to design and operate the activated sludge system under imposed effluent quality laws. We analyze four real world plants in the Trás-os-Montes region (Portugal) and report the numerical results obtained with the FILTER, IPOPT, SNOPT and LOQO optimizers.

1 Introduction

Wastewater treatment plants (WWTP's) are nowadays emerging everywhere as authorities concerned with environmental issues legislate tighter laws on water quality. The high costs associated with the plant installation and operation require a wise optimization of the process.

A typical WWTP is usually defined by a primary treatment, a secondary treatment and in some cases a tertiary treatment. The primary treatment is a physical process and aims to eliminate the gross solids and grease, so avoiding the blocking up of the secondary treatment. As its cost does not depend too much on the characteristics of the wastewater, we chose not to include it in the optimization procedure. The secondary treatment is a biological process and is the most important treatment in the plant because it eliminates the soluble pollutants. When the wastewater is very polluted and the secondary treatment does not provide the demanded quality, a tertiary treatment, usually a chemical process, can be included.

This paper is part of an ongoing research project in which we are engaged to optimize the design and the operation of WWTP's in terms of minimum total cost (investment and operation costs). The work herein presented focus solely on the secondary treatment, in particular on an activated sludge system, because this is the chosen secondary treatment to be used by the four plants that we propose to analyze - Alijó, Murça, Sabrosa de Aguiar and Sanfins do Douro -

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that are located in Trás-os-Montes region. This is a poor country region in the north of Portugal that produces high quality wines and has, besides domestic effluents, significant effluent variations in terms of amount of pollution and flow, during the vintage season. The mentioned system consists of an aeration tank and a secondary settler. The influent enters the aeration tank where the biological reactions take place, in order to remove the dissolved carbonaceous matter and nitrogen. The sludge that leaves this tank enters in the secondary settler to remove the suspended solids. After this treatment, the treated final effluent leaves the settling tank and the thickened sludge is recycled to the aeration tank and part of it is wasted.

The aim of this paper is to determine the optimal design and operation of the four above mentioned WWTP's, guaranteeing the water quality with pollution levels lower than the maxima defined by portuguese laws.

The optimal design and operation consists of finding the optimal aeration tank volume, sedimentation area and depth of the secondary settler tank, the air flow needed, to name a few, which yield the lowest total cost of the system.

The mathematical modelling of the system results in a smooth nonconvex nonlinear constrained optimization problem that is to be solved by NEOS Server (http://www-neos.mcs.anl.gov/neos/) optimization tools.

To the best of our knowledge, apart the work done by Tyteca et al. [5], that uses simple models to describe the aeration tank and the secondary settler, no WWTP real optimization has been published until now. Previous published work on activated sludge systems using ASM type models [4], [11] and, either the ATV [1] or the double exponential model [12] for settling tanks, focus on obtaining the best combination of the state variables testing by simulation two or three alternative designs and choosing the one with the lowest cost [8], [9], [10], [13]. The simulation is carried out using WEST++ (http://www.hemmis.be), GPS-X (http://www.hydromantis.com) and DESASS [8].

This paper is organized as follows. In Sect. 2 we present a not too much technical description of the equations of the mathematical model. Section 3 is devoted to the listing of some optimization tools in the NEOS Server for use to the public. Section 4 reports on the numerical experiments done on four real world problems and Sect. 5 contains the conclusions.

2 Mathematical Modelling

The system under study consists of an aeration tank, where the biological reactions take place, and a secondary settler for the sedimentation of the sludge and clarification of the effluent. To describe the aeration tank we chose the activated sludge model n.1, described by Henze et al. [4], which considers both the elimination of the carbonaceous matter and the removal of the nitrogen compounds. This model is widely accepted by the scientific community, as it produces good predictive values by simulations. This means that all state variables keep their biological interpretation. The tank is considered a completely stirred tank reactor (CSTR) in steady state. For the settling tank the ATV design procedure

[1] is used, which is a very simple model but describes the settling process very well, besides considering also peak flow events.

The problem contains seven sets of constraints. The first set results from mass balances around the aeration tank using the Peterson matrix of the ASM1 model [4]. The generic equation for a mass balance around a certain system considering a CSTR is

$$\frac{Q}{V_{\mathrm{a}}}\left(\xi_{\mathrm{in}}-\xi\right)+r_{\xi}=\frac{d\xi}{dt}\ ,$$

where Q is the flow that enters the tank, V_{a} is the aeration tank volume, ξ and ξ_{in} are the concentrations of the component around which the mass balances are being made inside the reactor and on entry, respectively. It is convenient to refer that in a CSTR the concentration of a compound is the same at any point inside the reactor and at the effluent of that reactor. The reaction term for the compound in question, r_{ξ}, is obtained by the sum of the product of the stoichiometric coefficients, $\nu_{\xi j}$, with the expression of the process reaction rate, ρ_j, of the ASM1 Peterson matrix [4]

$$r_{\xi}=\sum_{j}\nu_{\xi j}\rho_j\ .$$

In steady state, the accumulation term given by $\frac{d\xi}{dt}$ is zero, because the concentration is constant in time. A WWTP in labor for a sufficiently long period of time without significant variations can be considered at steady state. As our purpose is to make cost predictions in a long term basis it is reasonable to do so. The ASM1 model involves 8 processes incorporating 13 different components, such as the substrate, the bacteria, dissolved oxygen, among others. For the sake of clearness, we include here the mass balance equation related to one of the components - the soluble substrate (S_{S}):

$$\begin{aligned}\frac{-\mu_{\mathrm{H}}}{Y_{\mathrm{H}}}\frac{S_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{OH}}+S_{\mathrm{O}}}+\eta_{\mathrm{g}}\frac{K_{\mathrm{OH}}}{K_{\mathrm{OH}}+S_{\mathrm{O}}}\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}}+S_{\mathrm{NO}}}\right)X_{\mathrm{BH}}\\ +k_{\mathrm{h}}\frac{X_{\mathrm{BH}}}{K_{\mathrm{X}}X_{\mathrm{BH}}+X_{\mathrm{S}}}\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{OH}}+S_{\mathrm{O}}}+\eta_{\mathrm{h}}\frac{K_{\mathrm{OH}}}{K_{\mathrm{OH}}+S_{\mathrm{O}}}\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}}+S_{\mathrm{NO}}}\right)X_{\mathrm{S}}\\ +\frac{Q}{V_{\mathrm{a}}}\left(S_{\mathrm{S_{in}}}-S_{\mathrm{S}}\right)=0\ .\end{aligned}$$

We denote all the soluble components by $S_?$ and the particulates by $X_?$. All the other symbols are stoichiometric or kinetic parameters for the wastewater considered. (See [4] for details on how to obtain all the other equations.)

The second group of constraints concern the secondary settler and are set using the ATV procedure design [1]. Traditionally the secondary settler is underestimated when compared with the aeration tank. However, it plays a crucial role in the activated sludge system. When the wastewater leaves the aeration tank, where the biological treatment took place, the treated water should be separated from the biological sludge, otherwise, the chemical oxygen demand would be higher than it is at the entry of the system. The most common way of achieving this purpose is by sedimentation in tanks. The optimization of the sedimentation area and depth must rely on the sludge characteristics, which in turn are related with the performance of the aeration tank. So, the operation of the biological reactor influences directly the performance of the settling tank and for that reason, one should never be considered without the other. The ATV design procedure contemplates the peak wet weather flow (PWWF) events, during which there is a reduction in the sludge concentration. To turn around this problem, a certain depth is allocated to support the fluctuation of solids during these events ($h_3 = \varDelta X V_{\rm a}\frac{DVSI}{480A_{\rm s}}$). This way a reduction in the sedimentation area ($A_{\rm s}$) is allowed. A compaction zone ($h_4 = X_{\rm p}\frac{DVSI}{1000}$) , where the sludge is thickened in order to achieve the convenient concentration to return to the biological reactor, also has to be contemplated and depends only on the characteristics of the sludge. $DVSI$ is the diluted volumetric sludge index and $\varDelta X$ is the variation of the sludge concentration inside the aeration tank in a PWWF event. A clear water zone (h_1) and a separation zone (h_2) should also be considered and are set empirically ($h_1 + h_2 = 1$, say). The depth of the settling tank, h, is the sum of these four zones.

The sedimentation area is still related to the peak flow, $Q_{\rm p}$, by the expression

$$\frac{Q_{\rm p}}{A_{\rm s}} \le 2400\,(X_{\rm p}DVSI)^{-1.34} \quad .$$

The other important group of constraints are a set of linear equalities and define composite variables. In a real system, some state variables are, most of the time, not available for evaluation. Thus, readily measured composite variables are used instead. For example, the chemical oxygen demand (COD) is composed by soluble and particulate components, that are related by the equation

$$COD = S_{\rm I} + S_{\rm S} + X_{\rm I} + X_{\rm S} + X_{\rm BH} + X_{\rm BA} + X_{\rm P} \quad .$$

Similar equations can be defined for the volatile suspended solids (VSS), total suspended solids (TSS), biochemical oxygen demand (BOD), total nitrogen of Kjeldahl (TKN) and total nitrogen (N).

The system behavior, in terms of concentration and flows, may be predicted by balances. In order to achieve a consistent system, these balances must be done around the entire system and not only around each unitary process. They were done to the suspended matter, dissolved matter and flows and these correspond to the fourth group of constraints. The equations for particulate compounds (organic and inorganic) have the following form

$$(1+r)\,Q_{\rm inf}X_{?_{\rm ent}} = Q_{\rm inf}X_{?_{\rm inf}} + (1+r)\,Q_{\rm inf}X_{?} - \frac{V_{\rm a}X_{?}}{SRTX_{?_{\rm r}}}\left(X_{?_{\rm r}} - X_{?_{\rm ef}}\right) - Q_{\rm inf}X_{?_{\rm ef}}$$

and for the solubles we have

$$(1+r)\,Q_{\rm inf}S_{?_{\rm in}} = Q_{\rm inf}S_{?_{\rm inf}} + rQ_{\rm inf}S_{?_{\rm r}}$$

where r is the recycle rate, SRT is the sludge retention time and $Q_?$ represents the volumetric flows. As to the subscripts, inf concerns the influent wastewater, ent the entry of the aeration tank, r the recycled sludge and ef the treated effluent.

It is also necessary to add some system variables definitions, in order to define the system correctly. In this group we include the sludge retention time, the recycle rate, hydraulic retention time (HRT), recycle rate in a PWWF event (r_{p}), recycle flow rate in a PWWF event ($Q_{\mathrm{r_p}}$) and maximum overflow rate ($\frac{Q_{\mathrm{p}}}{A_{\mathrm{s}}}$):

$$SRT = \frac{V_{\mathrm{a}} X}{Q_{\mathrm{w}} X_{\mathrm{r}}}$$

$$HRT = \frac{V_{\mathrm{a}}}{Q}$$

$$r = \frac{Q_{\mathrm{r}}}{Q_{\mathrm{inf}}}$$

$$r_{\mathrm{p}} = \frac{0.7\, TSS}{TSS_{\mathrm{max_p}} - 0.7\, TSS}$$

$$Q_{r_{\mathrm{p}}} = r_{\mathrm{p}} Q_{\mathrm{p}}$$

$$\frac{Q_{\mathrm{p}}}{A_{\mathrm{s}}} \leq 2 \ .$$

A fixed value for the relation between volatile and total suspended solids was considered

$$\frac{VSS}{TSS} = 0.7 \ .$$

All the variables are considered nonnegative, although more restricted bounds are imposed to some of them due to operational consistencies. For example, the dissolved oxygen has to be always greater or equal to 2 mg/L. These conditions define a set of simple bounds on the variables.

Finally, the quality of the effluent has to be imposed. The quality constraints are usually derived from law restrictions. The most used are related with limits in the COD, N and TSS at the effluent. In mathematical terms, these constraints are defined by portuguese laws as $COD_{\mathrm{ef}} \leq 125$, $N_{\mathrm{ef}} \leq 15$ and $TSS_{\mathrm{ef}} \leq 35$.

The objective cost function used represents the total cost and includes both investment and operation costs. The operation cost is usually on annual basis, so it has to be updated to a present value using the adequate economic factors of conversion. Each term in the objective function is based on the basic model $C = aZ^b$ [5], where a and b are the parameters to be estimated, C is the cost and Z is the characteristic of the unitary process that most influences the cost. For example, for the investment cost of the aeration tank, the volume (V_{a}) and air flow (G_{S}) are considered. The parameters a and b are estimated by the least squares technique, using real data collected from a WWTP building company. The operation cost of the aeration tank considers the air flow, and the investment and operation costs of the secondary settler depend on the sedimentation area, A_s, and the depth, h. Summing up all these terms, we get the following objective cost function:

$$F_\mathrm{obj} = 174.2 V_\mathrm{a}^{1.07} + 12487 G_\mathrm{S}^{0.62} + 114.8 G_\mathrm{S} + 955.5 A_\mathrm{s}^{0.97} + 41.3 \left(A_\mathrm{s} h\right)^{1.07} \quad . \quad (1)$$

3 NEOS Server Usage

NEOS Server provides the possibility to run problems on powerful machines in a user friendly manner through the internet.

Depending on the type of optimization problem, the user has a list of solvers to choose from. The choice of solver is also dictated by the language used to define the optimization problem. Our problem was coded in AMPL format (http://www.ampl.com/cm/cs/what/ampl/).

The solvers for smooth nonlinear constrained optimization problems with AMPL input format are the following: FILTER, IPOPT, LOQO, SNOPT, KNITRO, LANCELOT, MINOS, MOSEK and PENNON.

From the list, we excluded immediately the MOSEK optimizer as it does not work for nonconvex problems. KNITRO, LANCELOT, MINOS and PENNON were also excluded because the first converged only for some of the carried out runs and the others did not converge at all. The remaining four optimizers converged in all runs although not all to the same solution. A brief description of each one follows.

FILTER is a software developed by R. Fletcher and S. Leyffer that is based on a Filter-SQP algorithm and implements a Sequential Quadratic Programming trust region algorithm with a filter to promote global convergence [2]. The idea of a filter is motivated by the aim of avoiding the need to use penalty parameters as required by l_1 or augmented Lagrangian merit functions.

IPOPT is an optimizer developed by A. Wächter, L. T. Biegler, A. Raghunathan and Yi-Dong Lang. It implements a primal-dual interior point algorithm with a filter line search strategy. As a barrier method, the algorithm computes approximate solutions for a sequence of barrier problems (associated with the original problem) for a decreasing sequence of positive barrier parameters converging to zero. The barrier problems are solved using a filter line search algorithm. We refer to the Technical Report [7] for details.

LOQO (http://www.princeton.edu/∼rvdb/loqo/) solver was developed by R. J. Vanderbei and H. Y. Benson, and it is based on an infeasible primal-dual interior point method with an l_2 penalty merit function to ensure progress toward feasibility and optimality [6].

SNOPT (http://www.sbsi−sol−optimize.com/asp/sol_product_snopt.htm) is a sequential quadratic programming method for large-scale optimization problems involving general linear and nonlinear constraints that uses an active-set approach [3].

We do not aim to analyze the performance of the solvers but rather to solve our design problem which, being a medium-scale problem, turns out to be a quite difficult one.

4 Computational Results

The problem of the optimal design and operation of the activated sludge system consists of finding the volume of the aeration tank, the air flow needed for the aeration tank, the sedimentation area, the secondary settler depth, the recycle rate, the effluent flow and concentration of total suspended solids, carbonaceous matter and total nitrogen in the treated water, to name a few, in such a way that, verifying the aeration tank balances as well as the system balances, satisfy the composite variables constraints, the secondary settler constraints, the system variables definition constraints, the quality constraints and the simple bounds on the variables, and minimize the cost function (1). Our formulated problem has 57 parameters, 82 variables and 64 constraints, where 28 are nonlinear equalities, 35 are linear equalities and there is only one nonlinear inequality. Seventy one variables are bounded below and eleven are bounded below and above. The chosen values for the stoichiometric, kinetic and operational parameters that appear in the mathematical formulation of the problem are the default values presented in the simulator GPS-X, and they are usually found in real activated sludge based plants for domestic effluents.

The collected data from the four analyzed small towns are listed in Table 1. These data consider the population equivalent, the influent flow, the peak flow, the influent COD, the influent TSS and define average conditions that are crucial for the dimensioning of the plant.

Table 1. Data collected from the four small towns

	Location of the WWTP			
	Alijó	Murça	Sabrosa	Sanfins
pop. eq.	6850	3850	2750	3100
influent flow (m^3/day)	1050	885	467.5	530
peak flow (m^3/h)	108	86.4	48.6	54
COD (Kg/m^3)	2000	1750	1250	1250
TSS (Kg/m^3)	750	660	610	610

Several experiences were done for the WWTP's under study, using the available NEOS Server solvers mentioned in Sect. 3, and considering different values of COD reduction in the preliminary treatment. This reduction typically varies from 40 to 70%. Table 2 presents the effect of the primary treatment efficiency on the cost of the activated sludge system for the WWTP from Alijó. The solver used was the FILTER. The values of the total cost are in millions of euros. In the table, we report the number of iterations needed by FILTER to converge to

Table 2. Comparison of the results in the WWTP from Alijó considering different COD reductions in the primary treatment

	COD reduction		
	40%	55%	70%
total cost	11.33	7.62	5.25
iterations	28	20	21
func. eval.	15	11	10
cons. eval.	34	20	21

Table 3. Results for the studied WWTPs for different solvers, considering 70% of COD reduction in the preliminary treatment

		Location of the WWTP			
Solver		Alijó	Murça	Sabrosa	Sanfins
FILTER	total cost	5.25	4.03	6.23	1.46
	iterations	21	20	19	40
	func. eval.	10	12	1	29
	cons. eval.	21	21	23	40
IPOPT	total cost	5.25	4.03	1.33	1.46
	iterations	53	50	68	63
	func. eval.	119	57	70	68
	cons. eval.	119	57	70	68
SNOPT 6.2	total cost	8.37	4.03	1.56	1.46
	iterations	346	529	853	665
	func. eval.	53	113	404	277
	cons. eval.	52	112	403	276
LOQO 6.06	total cost	8.36	5.91	1.56	1.70
	iterations	85	74	41	45
	func. eval.	85	74	41	45
	cons. eval.	85	74	41	45

the solution, the number of function evaluations and the number of constraints evaluations. As shown, the efficiency of a primary treatment is crucial because the higher is the achieved COD reduction, the lower is the investment and operation cost of the secondary treatment. We remark that the cost of the preliminary treatment is also related with its efficiency, although not as dramatic as the cost of the activated sludge system. Thus, for the remaining experiences we assume the most favorable situation, i.e., we assume that the preliminary treatment has an efficiency of 70%.

Table 3 reports on the minimum total cost (in millions of euros), of the four WWTP's under study, the number of iterations up to finding a solution and the number of function and constraints evaluations, using each one of the listed solvers. The solvers find the solutions using their default settings.

Table 4. Results of the optimal design and operation solution for the studied WWTPs considering 70% of COD reduction in the preliminary treatment

	Alijó	Murça	Sabrosa	Sanfins
$V_{\mathrm{a}}(\mathrm{m}^3)$	1673	1203	395	448
$A_{\mathrm{s}}(\mathrm{m}^2)$	217	173	97	108
$h(\mathrm{m})$	5.4	5.0	3.6	3.6
$G_{\mathrm{S}}(\mathrm{m}^3/\mathrm{day\,STP})$	8707	6039	1147	1300
$COD_{\mathrm{ef}}(\mathrm{g}\,COD/\mathrm{m}^3)$	98.8	99.6	125	125
$TSS_{\mathrm{ef}}(\mathrm{g}/\mathrm{m}^3)$	35.0	35	35	35
$N_{\mathrm{ef}}(\mathrm{g\,N}/\mathrm{m}^3)$	8.2	9.5	13.0	13.0

Some conclusions may be drawn. The solution found by each of the four solvers is not always the same. We also observe an overall advantage in using IPOPT optimizer as it converges to a solution with the lowest total cost in all plants.

Table 4 reports on optimal values of the aeration tank volume, sedimentation area, settler depth, air flow, chemical oxygen demand at the effluent, total suspended solids at the effluent and nitrogen at the effluent obtained by IPOPT optimizer for each plant. We remark that although the achieved values of TSS correspond to the imposed law limit, the same does not occur with COD and N.

The nitrogen that enters in the system is only the quantity requested to ensure the growth of the bacteria present in the biological sludge. This means that in this kind of populations the nitrogen levels are not considered pollutant. As it can be seen in Table 1, the nitrogen does not appear as an entering parameter. For that reason, the nitrogen at the effluent never reaches the limit imposed by law.

As to the COD we have a different situation. In the largest WWTP's (Alijó and Sanfins) the imposed law limit is not reached because to be able to achieve the TSS limit, the system is capable of removing more COD than the demanded. The opposite occurs in the other two plants. As they are very small, the minimum cost is achieved only when the COD reaches the limit.

5 Conclusions

In this paper we consider the optimal design and operation, in terms of minimum installation and operation cost, of an activated sludge system in WWTP's from the north of Portugal, based on portuguese real data and effluent quality law limits. Four real WWTP's were analyzed and the optimization of the problems was carried out running NEOS Server solvers (FILTER, IPOPT, LOQO and SNOPT).

From our numerical experiences, we may conclude that the efficiency of the primary treatment influences directly and in a very expressive way the resulting cost of the biological treatment. To have a more realistic idea of the best solution, the whole treatment plant should be considered as future developments.

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