How wastewater processes can be optimized using LOQO

I. A. C. P. Espírito-Santo¹, Edite M. G. P. Fernandes¹, M. M. Araújo¹, and E. C. Ferreira²

¹ Systems and Production Department, Minho University, Braga, Portugal
{iapinho;emgpf;mmaraujo}@dps.uminho.pt

² Centre of Biological Engineering, Minho University, Braga, Portugal
ecferreira@deb.uminho.pt

Summary. This paper describes the optimization of an activated sludge system which comprises an aeration tank and a secondary settler. This system is by far the most widely used biological process in wastewater treatment plants. The optimization process is represented as a smooth nonlinear problem with highly nonlinear equality constraints, some linear equality constraints, one inequality constraint and simple bounds, in which the objective is to minimize the total cost associated with the installation and operation of the biological process. We use the software LOQO to solve the problem. Several computational results show that the quality of the effluent, especially in terms of carbonaceous matter, influences directly the cost and the main contribution to the total cost is the air flow, due to the acquirement of the electromechanical equipment and spent energy.

1 Introduction

The optimization of natural processes is becoming nowadays more and more important. In the case of wastewater treatment plants (WWTPs), besides the simulation, which is quite common, see for example [9], it seems crucial to reduce, as much as possible, the costs associated with the design and operation of such plants, because they are so high that can threaten the very survival of many industries.

Besides the densely populated and industrial regions, it is also very important to treat the domestic effluents in small country regions. In particular, there is a small region in the north of Portugal, Trás-os-Montes, that produces high quality wines and has significant effluent variations in terms of amount of pollution and flow, during the vintage season.

A typical WWTP is schematically represented in Figure 1. The first three unit processes define the primary treatment which is a physical process and aims to eliminate the gross solids and grease, so avoiding the blocking up of the secondary treatment. Although the dimensioning of such units is usually

Fig. 1. Schematic representation of a typical WWTTP (Adapted from [10]).

empirical and based on the wastewater to be treated, its cost does not depend too much on the characteristics of the wastewater. This is the reason why this process is not included in the optimization procedure.

The next two units define the secondary treatment of the wastewater. It is the most important treatment in the plant because it eliminates the soluble pollutants. This is a biological process which, in the case herein studied, comprises an aeration tank and a clarifier and aims to separate the biological sludge from the treated water. There are other biological treatments but this is, by far, the most widely used.

Finally, the last unit is used to treat the biological sludge that is wasted by the secondary settler.

There are many other possible WWTTP layouts, but most of them have the above described treatments. 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 the whole plant 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 that is represented in Figure 2. This 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 where suspended solids are removed. 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.

For the case presented in this paper, the predominant costs related to the installation of a plant are concerned with the civil construction of the tanks and the acquirement of electromechanical equipment. The predominant

operation costs are due to the power required to the aeration of the activated sludge. The mathematical models used to describe the aeration tank and the settling tank are the ASM1 model [5] and the ATV model [2], respectively.

Fig. 2. Schematic representation of the activated sludge system (Adapted from the GPS-X simulator [6]).

This paper is organized as follows. In Section 2, we present the developed mathematical formulation of the problem. Section 3 contains details of the implementation of the resulting optimization problem and Sections 4 and 5 contain a brief discussion of the results and the conclusions.

2 The mathematical model

The mathematical model can be subdivided in seven types of equations, as it will be described. 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.* [5], 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 [2] is used, which is a very simple model but describes the settling process very well, besides considering also peak flow events.

2.1 Mass balances around the aeration tank

The first step in this unit process is to do mass balances around it, using the Peterson matrix of the ASM1 model [5].

The generic equation for a mass balance around a certain system is

In - Out + Reaction = Accumulation.

In mathematical language, for a CSTR

$$\frac{Q}{V_a} (\xi_{in} - \xi) + r_\xi = \frac{d\xi}{dt},$$

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 [5]

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

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. The mass balances for the inert materials, S_I and X_I , are not considered because they are transport-only components. All the symbols used in these formulae and throughout the paper are listed in the Appendix - Notation. The processes rates are the following:

Aerobic growth of heterotrophs, ρ_1

$$\rho_1 = \mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{OH} + S_O} \right) X_{BH};$$

Anoxic growth of heterotrophs, ρ_2

$$\rho_2 = \mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \eta_g X_{BH};$$

Aerobic growth of autotrophs, ρ_3

$$\rho_3 = \mu_A \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{OA} + S_O} \right) X_{BA};$$

Decay of heterotrophs, ρ_4

$$\rho_4 = b_H X_{BH};$$

Decay of autotrophs, ρ_5

$$\rho_5 = b_A X_{BA};$$

Ammonification of soluble organic nitrogen, ρ_6

$$\rho_6 = k_a S_{ND} X_{BH};$$

Hydrolysis of entrapped organics, ρ_7

$$\rho_7 = k_h \frac{\frac{X_S}{X_{BH}}}{K_X + \frac{X_S}{X_{BH}}} \left[\left(\frac{S_O}{K_{OH} + S_O} \right) + \eta_h \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right] X_{BH};$$

Hydrolysis of entrapped organic nitrogen, ρ_8

$$\rho_8 = \rho_7 \frac{X_{ND}}{X_S}.$$

The unit adopted for concentration is $g\ COD/m^3$ and the equations obtained from the ASM1 model with mass balances are as follows:

Soluble substrate (S_S)

$$-\frac{1}{Y_H} \rho_1 - \frac{1}{Y_H} \rho_2 + \rho_7 + \frac{Q}{V_a} (S_{S_{in}} - S_S) = 0; \quad (1)$$

Slowly biodegradable substrate (X_S)

$$(1 - f_P) \rho_4 + (1 - f_P) \rho_5 - \rho_7 + \frac{Q}{V_a} (X_{S_{in}} - X_S) = 0; \quad (2)$$

Heterotrophic active biomass (X_{BH})

$$\rho_1 + \rho_2 - \rho_4 + \frac{Q}{V_a} (X_{BH_{in}} - X_{BH}) = 0; \quad (3)$$

Autotrophic active biomass (X_{BA})

$$\rho_3 - \rho_5 + \frac{Q}{V_a} (X_{BA_{in}} - X_{BA}) = 0; \quad (4)$$

Particulate products arising from biomass decay (X_P)

$$f_P \rho_4 + f_P \rho_5 + \frac{Q}{V_a} (X_{P_{in}} - X_P) = 0; \quad (5)$$

Nitrate and nitrite nitrogen (S_{NO})

$$-\frac{1 - Y_H}{2.86 Y_H} \rho_2 + \frac{1}{Y_A} \rho_3 + \frac{Q}{V_a} (S_{NO_{in}} - S_{NO}) = 0; \quad (6)$$

$NH_4^+ + NH_3$ nitrogen (S_{NH})

$$-i_{X_B} \rho_1 - i_{X_B} \rho_2 - \left(i_{X_B} + \frac{1}{Y_A} \right) \rho_3 + \rho_6 + \frac{Q}{V_a} (S_{NH_{in}} - S_{NH}) = 0; \quad (7)$$

Soluble biodegradable organic nitrogen (S_{ND})

$$-\rho_6 + \rho_8 + \frac{Q}{V_a} (S_{ND_{in}} - S_{ND}) = 0; \quad (8)$$

Particulate biodegradable organic nitrogen (X_{ND})

$$(i_{X_B} - f_P i_{X_P}) \rho_4 + (i_{X_B} - f_P i_{X_P}) \rho_5 - \rho_8 + \frac{Q}{V_a} (X_{ND_{in}} - X_{ND}) = 0; \quad (9)$$

Alkalinity (S_{alk})

$$\begin{aligned} -\frac{i_{X_B}}{14} \rho_1 + \left(\frac{1 - Y_H}{14 \times 2.86 Y_H} - \frac{i_{X_B}}{14} \right) \rho_2 - \left(\frac{i_{X_B}}{14} + \frac{1}{7 Y_A} \right) \rho_3 + \frac{1}{14} \rho_6 \\ + \frac{Q}{V_a} (S_{alk_{in}} - S_{alk}) = 0; \end{aligned} \quad (10)$$

Oxygen (S_O)

$$K_L a (S_{O_{sat}} - S_O) - \frac{1 - Y_H}{Y_H} \rho_1 - \frac{4.57 - Y_A}{Y_A} \rho_3 + \frac{Q}{V_a} (S_{O_{in}} - S_O) = 0. \quad (11)$$

For oxygen mass transfer, the aeration by diffusion is considered:

$$K_L a = \frac{\alpha G_S \eta P_{O_2} 1333.3}{V_a S_{O_{sat}}} \theta^{(T-20)} \quad (12)$$

where

$$S_{O_{sat}} = \frac{1777.8 \beta \rho P_{O_2}}{Henry O_2}$$

and

$$\rho = 999.96(2.29 \times 10^{-2} T) - (5.44 \times 10^{-3} T^2), \quad Henry O_2 = 708 T + 25700.$$

2.2 Composite variables

In a real system, some state variables are, most of the time, not available from direct measurements. Thus, readily measured composite variables are used instead. They are defined as follows.

Particulate COD

$$X = X_I + X_S + X_{BH} + X_{BA} + X_P; \quad (13)$$

Soluble COD

$$S = S_I + S_S; \quad (14)$$

Total COD

$$COD = X + S; \quad (15)$$

Volatile suspended solids

$$VSS = \frac{X}{icv}; \quad (16)$$

Total suspended solids

$$TSS = VSS + ISS; \quad (17)$$

Biochemical oxygen demand

$$BOD = f_{BOD} (S_S + X_S + X_{BH} + X_{BA}); \quad (18)$$

Total nitrogen of Kjeldahl

$$TKN = S_{NH} + S_{ND} + X_{ND} + i_{XB} (X_{BH} + X_{BA}) + i_{XP} (X_P + X_I); \quad (19)$$

Total nitrogen

$$N = TKN + S_{NO}. \quad (20)$$

2.3 Quality constraints

Quality constraints are usually derived from environmental law restrictions. The most used are related with limits in the chemical oxygen demand (COD), total nitrogen (N), and total solids (TSS) at the effluent. In mathematical terms, these constraints are defined as:

$$COD_{ef} \leq COD_{law} \quad (21)$$

$$N_{ef} \leq N_{law} \quad (22)$$

$$TSS_{ef} \leq TSS_{law}. \quad (23)$$

2.4 Constraints of the secondary settler

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 COD 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.

A good settler tank has to accomplish three different functions. As a thickener, it aims to produce a continuous underflow of thickened sludge to return to the aeration tank; as a clarifier, it produces a good quality final effluent and as a storage tank it allows the conservation of the sludge in peak flow events. None of these functions could fail. If that happens the effluent will be of poor quality and the overall behavior of the system can be compromised.

The behavior of a settling tank depends on its design and operation, namely the hydraulic features, as the flow rate, the physical features, as inlet

and sludge collection arrangements, site conditions, as temperature and wind, and sludge characteristics. The factors that most influence the size of the tank are the wastewater flow and the characteristics of the sludge. As the former is known, 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, in which the sludge mass transferred from the biological reactor is ΔXV_a , where ΔX is the change in the sludge concentration within the aeration tank. A reduction of 30% on the sludge concentration for a PWWF event is considered. A higher reduction of the sludge concentration into the biological reactor may compromise the entire process.

Fig. 3. Typical solids concentration-depth profile adopted by the ATV design procedure (Adapted from [2]).

A way of turning around this problem is to allocate a certain depth (h_3 from Figure 3) to support the fluctuation of solids during these events. Thus, the sludge storage depth depends on the mass that needs to be stored during a PWWF and is given by

$$h_3 = \Delta XV_a \frac{DSVI}{480A_s}. \quad (24)$$

When this zone is considered, a reduction in the sedimentation area is allowed.

The transferred sludge causes the biological sludge concentration in the reactor at PWWF to decline, which allows a higher overflow rate and therefore a smaller surface area. However, the greater the decrease in reactor concentration is, the greater is the mass of sludge to be stored in the settler tank, so the deeper the tank needs to be. The ATV procedure allows a trade-off between surface area and depth and one may select the area/depth combination that suites the particular site under consideration. As the work herein presented aims to reduce costs, both the surface area and depth are considered as variables and the combination goals for the minimum cost.

The compaction zone, h_4 , where the sludge is thickened in order to achieve the convenient concentration to return to the biological reactor, depends only on the characteristics of the sludge, and is given by

$$h_4 = X_p \frac{DSVI}{1000} \quad (25)$$

where X_p is the sludge concentration in the biological reactor during a PWWF event.

The clear water zone, h_1 , and the separation zone, h_2 , are set empirically, in our case to $0.5m$. The depth of the settling tank, h , is the sum of these four zones, and should not be less than $2m$.

The sedimentation area is still related to the peak flow, Q_p , by the expression

$$\frac{Q_p}{A_s} \leq 2400 (X_p DSVI)^{-1.34} \quad (m/h). \quad (26)$$

2.5 Flow and mass balances around the system

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.

In the case of the suspended matter, the mass balances concern the organic (X) and inorganic (X_{II}) solids :

$$(1+r) Q_{inf} X_{in} = Q_{inf} X_{inf} + (1+r) Q_{inf} X - \frac{V_a X}{SRT X_r} (X_r - X_{ef}) - Q_{inf} X_{ef} \quad (27)$$

$$Q_{inf} 0.2 TSS_{inf} = \frac{V_a X_{II}}{SRT X_r} (X_{II,r} - X_{II,ef}) + Q_{inf} X_{II,ef}. \quad (28)$$

The balances of the dissolved matter are done for each one of the dissolved components:

$$(1+r) Q_{inf} S_{S_{in}} = Q_{inf} S_{S_{inf}} + r Q_{inf} S_{S_r}. \quad (29)$$

$$(1+r) Q_{inf} S_{O_{in}} = Q_{inf} S_{O_{inf}} + r Q_{inf} S_{O_r} \quad (30)$$

$$(1+r) Q_{inf} S_{NO_{in}} = Q_{inf} S_{NO_{inf}} + r Q_{inf} S_{NO_r} \quad (31)$$

$$(1+r) Q_{inf} S_{NH_{in}} = Q_{inf} S_{NH_{inf}} + r Q_{inf} S_{NH_r} \quad (32)$$

$$(1+r) Q_{inf} S_{ND_{in}} = Q_{inf} S_{ND_{inf}} + r Q_{inf} S_{ND_r} \quad (33)$$

$$(1+r) Q_{inf} S_{alk_{in}} = Q_{inf} S_{alk_{inf}} + r Q_{inf} S_{alk_r} \quad (34)$$

Besides the mass balances, flow balances are also necessary:

$$Q = Q_{inf} + Q_r \quad (35)$$

$$Q = Q_{ef} + Q_r + Q_w. \quad (36)$$

2.6 Simple bounds

All variables must be nonnegative, although more restricted bounds are imposed to some of them due to operational consistencies, namely:

$$\begin{aligned} 0 &\leq K_L a \leq 300 & 0.05 &\leq HRT \leq 2 \\ 800 &\leq TSS \leq 6000 & 0.5 &\leq r \leq 2 \\ 2500 &\leq TSS_r \leq 10000 & 6 &\leq S_{alk} \leq 8 \\ 6 &\leq S_{alk_{in}} \leq 8 & S_O &\geq 2 \end{aligned} \quad (37)$$

2.7 System variables definition

To complete the model, some definitions are added:

Sludge retention time

$$SRT = \frac{V_a X}{Q_w X_r}; \quad (38)$$

Hydraulic retention time

$$HRT = \frac{V_a}{Q}; \quad (39)$$

Recycle rate

$$r = \frac{Q_r}{Q_{inf}}; \quad (40)$$

$$r = \frac{TSS}{TSS_{r_{max}} - TSS}; \quad (41)$$

Recycle rate in a PWWF event

$$r_p = \frac{0.7 TSS}{TSS_{max_p} - 0.7 TSS}; \quad (42)$$

Recycle flow rate during a PWWF event

$$Q_{r_p} = r_p Q_p; \quad (43)$$

Maximum overflow rate

$$\frac{Q_p}{A_s} \leq 2. \quad (44)$$

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

$$\frac{VSS}{TSS} = 0.7. \quad (45)$$

2.8 The objective cost function

The cost function represents the total cost and includes both investment and operation costs. In this paper, for the sake of simplicity, no pumps were considered, which means that all the flows in the system move by the effect of gravity.

The operation cost is usually on annual basis, so it has to be updated to a present value with the updating term Γ :

$$\Gamma = \sum_{j=1}^n \frac{1}{(1+i)^j} = \frac{1 - (1+i)^{-n}}{i}, \quad (46)$$

where i is the discount rate and n is the life span of the WWTP. We use $i = 0.05$ and $n = 20$ years. The total cost is given by the sum of the investment (IC) and operation (OC) costs:

$$TC = IC + OC.$$

To obtain a cost function based on portuguese real data, a study was carried out with a WWTP building company. The basic structure of the model is $C = aZ^b$ [7], where a and b are the parameters to be estimated and Z is the characteristic of the unit process that most influences the cost. This model is nonlinear in the parameters, but it can be easily linearized. The obtained linear model is

$$\ln C = \ln a + b \ln Z$$

and the parameters $\ln a$ and b are estimated by the least squares technique.

The real data collected from the portuguese company are presented in Tables 1 and 2.

The investment cost function obtained for the aeration tank is

$$IC_a = 148.6V_a^{1.07} + 7737G_S^{0.62}.$$

The collected data come from a set of WWTPs in design, thus operation data are not available. However, from the company experience, the maintenance expenses for the civil construction are around 1% of the investment costs

Table 1. Real data obtained for the aeration tank

V_a (m^3)	G_S (m^3/day STP)	HP ($KW.h$) (annual basis)	$Cost(euro)$	
			Civil construction	Electromechanical
400	437	27720	87158	8416
600	597	129600	159796	10029
1000	943	95040	189952	12199
1300	1283	162000	366146	17056

Table 2. Real data obtained for the secondary settler

A_s (m^2)	h (m)	V_s (m^3)	$Cost$ (euro)
51.8	3.55	184	39355
71.4	3.9	278	61348
100	4.55	455	103741

during the first 10 years and around 2% otherwise. For the electromechanical components, the maintenance expenses are negligible, but all the materials are usually replaced after 10 years. The energy cost is directly related with the air flow. The second value in Table 1 was not used in our estimation because in this plant the planned air flow was in excess for some reason. The power cost (P_c) in Portugal is 0.08 *euro/KW.h*. With this information and with the updating term Γ (46), the operation cost of the aeration tank is then

$$OC_a = \left[0.01\Gamma + 0.02\Gamma(1+i)^{-10} \right] (148.6V_a^{1.07}) + (1+i)^{-10} 7737G_S^{0.62} + 115.1\Gamma P_c G_S.$$

The term $(1+i)^{-10}$ is used to bring to present a future value, in this case, 10 years from now.

The settling tank was considered to operate only by gravity. Thus, with the data from Table 2 and adopting the same mathematical procedure, the correspondent investment cost function is

$$IC_s = 955.5A_s^{0.97}$$

and for the operation cost function, that only concerns the maintenance for the civil construction,

$$OC_s = \left[0.01\Gamma + 0.02\Gamma(1+i)^{-10} \right] (148.6(A_s h)^{1.07}).$$

The total cost function is given by the sum of all the functions previously presented:

$$TC = 174.2V_a^{1.07} + 12487G_S^{0.62} + 114.8G_S + 955.5A_s^{0.97} + 41.3[A_s(1+h_3+h_4)]^{1.07}. \quad (47)$$

3 Numerical resolution

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 (1-12) and system balances (27-36), satisfy the composite variables constraints (13-20), the secondary settler constraints (24-26), the system variables constraints (38-45), the quality constraints (21-23) and the bounds (37), and minimize the cost function (47). This problem has 57 parameters, 82 variables and 64 constraints, where 28 are nonlinear equalities, 1 is a nonlinear inequality and 35 are linear equalities. Seventy one variables are bounded below and eleven are bounded below and above. Table 3 lists all the variables involved, as well as the initial values supplied to the solver.

Table 3. Variables of the problem and their initial values

Variable	init. val.	Variable	init. val.	Variable	init. val.	Variable	init. val.
Q	4000	$X_{BH_{in}}$	0	$X_{ND_{in}}$	0	VSS_r	0
Q_w	100	X_{BH}	350	X_{ND}	20	VSS_{ef}	0
Q_r	2000	X_{BH_r}	711	X_{ND_r}	0	TSS_{in}	0
Q_{ef}	1900	$X_{BH_{ef}}$	0	$X_{ND_{ef}}$	0	TSS	1800
Q_{r_p}	0	$X_{S_{in}}$	0	K_{La}	100	TSS_r	5000
r	1	X_S	350	G_S	10000	TSS_{ef}	10
V_a	1000	X_{S_r}	807	X_{in}	0	X_{II}	0
A_s	1000	$X_{S_{ef}}$	0	X	1000	$X_{II_{ef}}$	0
h_3	0	$X_{BA_{in}}$	0	X_r	4440	X_{II_r}	0
h_4	0	X_{BA}	10^{-6}	X_{ef}	0	BOD_{in}	0
r_p	0	X_{BA_r}	2×10^{-6}	S_{in}	0	BOD	500
X_I	727	$X_{BA_{ef}}$	0	S	50	BOD_r	0
X_{I_r}	950	$S_{NH_{in}}$	0	$S_{alk_{in}}$	0	BOD_{ef}	0
$X_{I_{ef}}$	0	S_{NH}	7.5	S_{alk}	7	TKN_{in}	0
SS_{in}	0	$X_{P_{in}}$	0	COD_{in}	0	TKN	106
SS	10	X_P	90	COD	1600	TKN_r	0
SO	2	X_{P_r}	175	COD_r	0	TKN_{ef}	0
SO_{in}	0	$X_{P_{ef}}$	0	COD_{ef}	0	N_{in}	0
SNO_{in}	0	$S_{ND_{in}}$	0	VSS_{in}	0	N_r	0
SNO	10^{-6}	S_{ND}	0.5	VSS	1050	N_{ef}	0
HRT	3.5	N	106				

In Tables 4 to 7, we summarize the data parameter chosen to obtain the results of Section 4. These values are as the default values presented in the GPS-X simulator [6], and are usually found in the real activated sludge based

plants for domestic effluents. The remaining parameters are defined as functions of the already listed parameters.

This problem was coded in the AMPL language [3] and the results were obtained running the solver LOQO V6.06 (<http://www.princeton.edu/~rvdb/loqo/>), an infeasible primal-dual interior point method [8]. In the stopping rule, we considered primal and dual infeasibilities $\leq 10^{-5}$ and 2 digits of agreement between the primal and dual objective functions. All the other adjustable LOQO parameters were left as default.

Table 4. Stoichiometric parameters

Parameter	Value	Parameter	Value
Y_A	0.24	i_{X_B}	0.086
Y_H	0.666	i_{X_P}	0.06
f_P	0.08		

Table 5. Kinetic parameters

Parameter	Value	Parameter	Value
μ_H	6	k_h	3
K_S	20	K_X	0.03
K_{OH}	0.2	μ_A	0.8
K_{NO}	0.5	K_{NH}	1
b_H	0.62	b_A	0.04
η_g	0.8	K_{OA}	0.4
η_h	0.4	k_a	0.08

Table 6. Operational parameters

Parameter	Value	Parameter	Value
T	20	α	0.8
P_{O_2}	0.21	η	0.07
$DSVI$	150	Q_p	150
SRT	20	β	0.95
θ	1.024		

Table 7. Characteristics of the influent to the system

Parameter	Value	Parameter	Value
Q_{inf}	2000	$X_{I,inf}$	73.65
$S_{I,inf}$	30	$X_{S,inf}$	123
$X_{BH,inf}$	0	$S_{NH,inf}$	11.7
$X_{BA,inf}$	0	$S_{ND,inf}$	0.63
$X_{P,inf}$	0	$X_{ND,inf}$	1.251
$S_{O,inf}$	0	$X_{II,inf}$	59.6
$S_{NO,inf}$	0	X_{inf}	196.7
$S_{alk,inf}$	7	S_{inf}	82.73
$S_{S,inf}$	52.73		

4 Discussion

Several experiments were done for different values of the required COD at the effluent, considering 15 g/m^3 as the N concentration limit and 35 g/m^3 as the TSS concentration limit, at the effluent. The COD limits vary from 45, that is the lowest value with which convergence was obtained, till 140. The value imposed by the portuguese environmental law is 125. The problem does not converge for smaller values of COD_{law} because there is a minimum under which it is not possible to treat the effluent more, due to the inert contribution (S_I), which is not possible to eliminate with a biological process, from the total COD .

The solution values of the most important variables, such as the total suspended solids and total nitrogen at the effluent, the aeration tank volume, the sedimentation area and depth of the secondary settler, the demanded air flow, the recycle rate, the effluent flow and the total cost are reported in Table 8, for different values of the imposed COD limit (COD_{law}). The number of iterations used by LOQO to converge to the solution, according to the previously defined stopping rule, is shown in the last column of the table.

For an easier interpretation of the results, two graphics were constructed. Figure 4 maps the total cost and the value of the quality index (QI) [1], which defines the amount of pollution at the final effluent, as function of the imposed COD limit. Figure 5 compares the contributions of investment/operation costs and aeration tank/secondary settler costs.

As it can be observed from Table 8 and Figure 4, the total cost decreases and the quality of the effluent deteriorates as the imposed COD at the effluent increases. In terms of total cost, the reduction is more pronounced for COD limits between 45 and 85. For $COD_{law} = 85$ and over the observed cost reduction is very small. For example, when $COD_{law} = 85$ the attained minimum cost is 1.4 millions of euros whereas for $COD_{law} = 125$ the minimum cost decreases to 1.3 millions of euros. This is due to the operational limits and from a certain point on the project cost can no longer decrease.

Table 8. Results for some of the variables for $N_{law} = 15$ and $TSS_{law} = 35$

COD_{l3w} (g/m^3)	TSS_{cf} (g/m^3)	N_{cf} (g/m^3)	V_a m^3	A_s m^2	h (m)	G_S (m^3/d STP)	r	Q_{cf} (m^3/d)	Total cost 10^6 euros	LOQO iterations
45	0.40	5.9	1346	337	3.5	14521	1.8	1933	7.2	86
50	0.16	9.0	1483	332	3.7	8735	1.8	1929	5.3	72
55	1.8	10.2	1525	330	3.7	6320	1.8	1931	4.4	75
60	1.8	11.0	1498	341	3.7	4796	1.9	1931	3.8	75
65	0.93	11.7	1462	351	3.6	3629	2.0	1931	3.2	89
70	0.50	12.2	1454	351	3.6	2641	2.0	1930	2.8	92
75	0.32	12.4	1444	351	3.6	1755	2.0	1932	2.3	100
80	0.15	12.7	1431	351	3.6	933	2.0	1929	1.8	113
85	1.6	13.1	1408	351	3.6	503	2.0	1930	1.4	84
90	4.9	13.2	1373	351	3.5	503	2.0	1930	1.4	71
95	8.3	13.3	1338	351	3.5	503	2.0	1935	1.4	52
100	11.7	13.6	1303	351	3.4	503	2.0	1932	1.4	54
105	15.1	13.9	1268	351	3.4	503	2.0	1933	1.4	55
110	18.4	14.1	1233	351	3.3	503	2.0	1934	1.4	61
115	21.8	14.2	1197	351	3.3	503	2.0	1942	1.3	67
120	25.2	14.3	1162	351	3.2	503	2.0	1941	1.3	59
125	28.7	14.4	1136	347	3.2	503	2.0	1941	1.3	110
130	32.3	14.4	1117	340	3.1	503	1.9	1946	1.3	209
135	35.0	14.5	1099	334	3.1	503	1.8	1948	1.3	266
140	35.0	14.5	1099	334	3.1	503	1.8	1946	1.3	271

Fig. 4. Total cost (TC) and quality index (QI) versus COD limit at the effluent.

Regarding the quality index, it deteriorates more stressfully until a COD limit of 60. For higher values the deterioration of the effluent grows almost linearly.

Another important observation is that although the COD limit is always achieved, TSS only reaches its limit when the COD limit is 135 and over, and the N limit is never attained. Nevertheless, as the imposed COD limit increases, the TSS and N at the effluent get larger. This means that for the considered interval, the carbonaceous matter dominates the process, being the parameter that determines the cost.

For COD limit values between 90 and 120, the sedimentation area is maintained at $351 m^2$ while the depth decreases because, as mentioned in Subsection 2.4, this model allows a trade-off between the sedimentation area and the settler depth. However, the five cases displayed with $A_s = 351$ and $h = 3.6$ are

Fig. 5. Contributions of investment/operation costs and aeration tank/secondary settler costs.

acceptable because the TSS concentrations are kept very small. For higher imposed COD limits, both sedimentation area and depth decrease.

The aeration tank volume and the air flow generally decrease as the imposed COD limit increases. From the dramatic reduction of the air flow verified for the COD limit interval $[45, 85]$, we may conclude that the air flow is the main contribution to the total cost.

As to the recycle rate, it reaches 2 (its maximum value) at a $COD_{law} = 65$, and this happens for two reasons. First, to get the minimum of TSS at the effluent, the sludge goes to the underflow. Second, to achieve the demanded quality it is necessary to keep as much biomass as possible inside the aeration tank.

Now, looking into the costs with more detail, from Figure 5 we can see that the investment costs overlap the operation costs, for a life span of 20 years. However, for a more demanding system this difference is smaller. For example, with a $COD_{law} = 45$, the operation costs equal the investment costs. Regarding the two involved unit processes, we may conclude that the cost associated with the aeration tank is much higher than that of the secondary settler, in particular for COD_{law} values smaller than 85. In both cases, the relations between costs are maintained almost constant for COD_{law} values of 85 and higher.

5 Conclusions

In this paper we present the mathematical formulation of a nonlinear problem that considers the optimal design and operation, in terms of minimum installation and operation cost, of an activated sludge system in WWTP's, based on

portuguese real data and effluent quality law limits. The optimization process was carried out running LOQO.

From our numerical experience we may conclude that the quality of the effluent influences directly the cost of the treatment plant project, especially in terms of carbonaceous matter (*COD*). With the environmental law invigorating in Portugal, only the *COD* limit influences the cost of the design. With the compelling observance of portuguese environmental law, neither *TSS* nor *N* reach their legal limits, 35 and 15 respectively, when the $COD_{ef} = 125$.

The main contribution to the total cost is the air flow because it influences the design in the project (electromechanical material) and during the operation (consumption of energy by the aeration).

Our next task is to add an anoxic preliminary treatment for phosphorous removal in series with the aeration tank, that may be described by the model ASM2d [4], and to reoptimize the process.

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Appendix - Notation

The following symbols are used in this paper:

- b_A =decay coefficient for autotrophic biomass, day^{-1}
 b_H =decay coefficient for heterotrophic biomass, day^{-1}
 BOD =biochemical oxygen demand, $g\ O_2/m^3$
 BOD_U =ultimate BOD , $g\ O_2/m^3$
 COD =chemical oxygen demand, $g\ COD/m^3$
 $DSVI$ =Diluted sludge volume index
 f_{BOD} = BOD/BOD_U ratio
 f_P =fraction of biomass leading to particulate products
 G_S =air flow rate, m^3/day at STP
 $HenryO_2$ =Henry constant
 HRT =hydraulic retention time, day
 i =discount rate
 $icv=X : VSS$ ratio, $g\ COD/g\ VSS$
 i_{XB} =nitrogen content of active biomass, $g\ N/g\ COD$
 i_{XP} =nitrogen content of endogenous/inert biomass, $g\ N/g\ COD$
 IC =investment cost, 2003 *euros*
 ISS =inorganic suspended solids, g/m^3
 k_a =ammonification rate, $m^3/g\ COD/day$
 k_h =maximum specific hydrolysis rate, day^{-1}
 K_{La} =overall mass transfer coefficient, day^{-1}
 K_{NH} =ammonia half-saturation coefficient for autotrophic biomass growth, $g\ N/m^3$
 K_{NO} =nitrate half saturation coefficient for denitrifying heterotrophic biomass, $g\ N/m^3$
 K_{OA} =oxygen half-saturation coefficient for autotrophs growth, $g\ O_2/m^3$
 K_{OH} =oxygen half-saturation coefficient for heterotrophs growth, $g\ O_2/m^3$
 K_S =readily biodegradable substrate half-saturation coefficient for heterotrophic biomass, $g\ COD/m^3$
 K_X =half-saturation coefficient for hydrolysis of slowly biodegradable substrate, $g\ COD/g\ COD$

n =life span of the treatment plant, *years*
 N =total nitrogen, $g\ N/m^3$
 OC =operation costs, 2003*euros*
 P_{O_2} =partial pressure of oxygen uncorrected
 $PWWF$ =Peak wet weather flow
 Q =flow, m^3/day
 QI =quality index, $Kg\ of\ pollution/day$
 r =recycle rate
 S =soluble COD, $g\ COD/m^3$
 S_{alk} =alkalinity, molar units
 S_I =soluble inert organic matter, $g\ COD/m^3$
 S_{ND} =soluble biodegradable organic nitrogen, $g\ N/m^3$
 S_{NH} =free and ionized ammonia, $g\ N/m^3$
 S_{NO} =nitrate and nitrite nitrogen, $g\ N/m^3$
 S_O =dissolved oxygen, $g\ (-COD)/m^3$
 $S_{O_{sat}}$ =saturated oxygen concentration, g/m^3
 S_S =readily biodegradable soluble substrate, $g\ COD/m^3$
 SRT =sludge retention time, *day*
 STP =standard temperature and pressure
 TC =total costs, 2003*euros*
 V_a =aeration tank volume, m^3
 VSS =volatile Suspended Solids, g/m^3
 T =temperature, $^{\circ}C$
 TKN =total nitrogen of Kjeldahl, $g\ N/m^3$
 TSS =total Suspended Solids, g/m^3
 X =particulate COD, $g\ COD/m^3$
 X_{BA} =active autotrophic biomass, $g\ COD/m^3$
 X_{BH} =active heterotrophic biomass, $g\ COD/m^3$
 X_I =particulate inert organic matter, $g\ COD/m^3$
 X_{II} =inert inorganic suspended solids, g/m^3
 X_{ND} =particulate biodegradable organic nitrogen, $g\ N/m^3$
 X_P =particulate products arising from biomass decay, $g\ COD/m^3$
 X_S =slowly biodegradable substrate, $g\ COD/m^3$
 Y_A =yield for autotrophic biomass, $g\ COD/g\ N$
 Y_H =yield for heterotrophic biomass, $g\ COD/g\ COD$
 α =wastewater/clean water coefficient
 β =salts and ions correction factor
 η =standard oxygen transfer efficiency
 η_g =correction factor for μ_H under anoxic conditions
 η_h =correction factor for hydrolysis under anoxic conditions
 μ_A =maximum specific growth rate for autotrophic biomass, day^{-1}
 μ_H =maximum specific growth rate for heterotrophic biomass, day^{-1}
 ρ =density of water, Kg/m^3
 θ =temperature correction factor

subscripts

a=aeration tank

ef=effluent

in=entry of the aeration tank

inf=influent

p=during a PWWF event

r=recycle

s=settling tank

w=sludge waste

no index=inside the aeration tank=exit of the aeration tank