AN OPTIMAL CONTROL PROBLEM APPLIED TO A WASTEWATER TREATMENT PLANT

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Abstract. This paper aims to present a mathematical model that describes the operation of an activated sludge system during one day. Such system is used in the majority of wastewater treatment plants and depends strongly on the dissolved oxygen, since it is a biological treatment. To guarantee the appropriate amount of dissolved oxygen, expensive aeration strategies are demanded, leading to high costs in terms of energy consumption. It was considered a typical domestic effluent as the wastewater to test the mathematical model and it was used the ASM1 to describe the activated sludge behaviour. An optimal control problem was formulated whose cost functional considers the trade-off between the minimization of the control variable herein considered (the dissolved oxygen) and the quality index that is the amount of pollution. The optimal control problem is treated as a nonlinear optimization problem after discretization by direct methods. The problem was then coded in the AMPL programming language in order to carry out numerical simulations using the NLP solver IPOPT from NEOS Server.

1. **Introduction.** Nowadays, with the increasing of environmental consciousness, it is crucial to treat wastewaters efficiently, without disregarding economic concerns, since treating wastewater is a very expensive process that can alone threaten the economic survival of small towns. When considering a wastewater treatment plant (WWTP) based on an activated sludge system, the most significant cost is related to the oxygen consumption that is directly related to the amount of dissolved oxygen in the sludge, where the microorganisms responsible for the pollutants removal are present. It is fundamental to maintain the level of oxygen that is necessary to assure the correct growth and maintenance of the aerobic bacteria present in the sludge, that guarantee the required level of treatment of the wastewater, but aerating the sludge demands large amounts of energy to operate de aeration pumps.

In [19], it is proposed a strategy of control optimization to achieve a reduction in greenhouse gas emissions, from a multi-objective point of view. Operational costs and amount of pollution are also considered as objectives to minimize. These

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are the focus in the work herein presented, where the dissolved oxygen is used as control since it is the main contribution to the activated sludge system operation costs and it is more readily available. Similarly, in both works legislative compliance is imposed.

In [15] a more practical approach is presented, with a controller measuring dissolved oxygen and nitrogen concentrations on-line, predicting immediate future scenarios that are continually adjusted. Our approach is in this phase more theoretical in order to provide guidelines to an activated sludge system operation during one day. Hreizab *et.al* [13] also proposes a multi-objective dynamic optimization, but in this case a very particular case is explored, in which is considered a reduction of the operation costs due to the incineration of the sludge. Although it seems very interesting, this paper is limited to the presented case, whereas our work addresses a problem that can be more widely used.

The concern of the work presented in [1] is also to control the aeration process in order to reduce the operation costs. However, it is based on simulations rather than on a true optimization procedure. In [9] a genetic algorithm is used to solve a multi-objective problem. The water quality indicators are used as control objectives. However, it can be difficult to actually use it as control as it is hard to restrain the quality of the wastewater entering in a WWTP. On the other hand, in our work the dissolved oxygen is used as control, which is much easier to implement in a real system.

Holenda *et al.* [12] also apply a genetic algorithm, alternating aerobic (providing oxygen) and anoxic (not providing oxygen) conditions, switching aeration sequentially on and off. The aim, however, is to minimize the pollution load of the treated water, rather than any kind of operational costs, which seems fairly unrealistic. A similar strategy is proposed in [7] where the optimal sequence of aeration/non-aeration times is determined to keep the effluent constraints feasible, maintaining the plant in cyclic steady-state. Also in [4] a set of aerators working on/off are considered, proposing a hybrid non-linear predictive control algorithm.

In the present work the ideal dissolved oxygen in each day (24 hours interval) is obtained. This allows to perceive in a very in-depth way each of the studied scenarios to be possible then to make effective suggestions in a real activated sludge system.This trade-off between the quality of the treated water, measured by a Quality Index (QI), and the consumption of oxygen, that will provide the dissolved oxygen (S_O) to the bacteria, suggests the formulation of an optimal control problem. This nonlinear optimization problem has an objective function and a set of constraints. The function to optimize includes two goals simultaneously – the dissolved oxygen and the quality of the treated water (QI) – using weights for each of them. The constraints are a set of ordinary differential equations related to the balances in the aeration tank, and some equalities and inequalities. We remark that the amount of dissolved oxygen in the sludge depends directly on the oxygen provided through aeration pumps present in the aeration tank, that can be turned on/off by controllers. The optimal control problem will be solved using a direct method, discretizing the differential equations by Euler's method.

The activated sludge system is composed by an aeration tank, where the biological reactions take place, and a secondary settler, where the sludge is separated from the treated water before it leaves the system. For the sake of simplicity, the settler in this work is considered a simple point of separation (non-dimensional), since the focus here is the optimal control of the aeration in the aeration tank (Figure 1). As

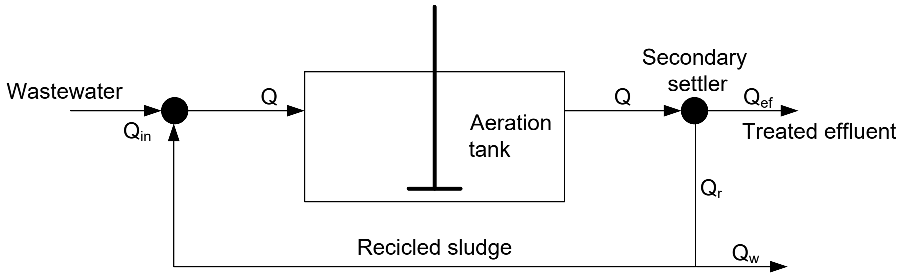


FIGURE 1. Schematic view of the activated sludge system.

to the aeration tank, the ASM1 model [10] is used, due to its universal appeal in the scientific community.

This research has two main objectives, firstly to analyze the level of quality of the treated water and at the same time, to understand the economic impact of the control of the dissolved oxygen in the maintenance of the quality of the treated water.

The work is organized in six main sections, as outlined next. The mathematical model is presented in Section 2. Then, the information related to the optimal control problem in order to study the impact of quality index and oxygen level is shown in Section 3. The methodology used to solve this simulation problem is described in Section 4. The computational results of several simulations are compiled in Section 5. Finally, the main conclusions are given in Section 6.

2. Mathematical model.

The generic mathematical mass balance, considering a CSTR (Completed Stirred Tank Reactor) is given by

$$\frac{d\xi}{dt} = \frac{Q}{V_a}(\xi_{\text{in}} - \xi) + r_\xi \tag{1}$$

being Q the volumetric flow, V_a is the aeration tank volume, ξ is the concentration of the compound around which the balances are made, ξ_{in} is the concentration of the compound at the entry of the aeration tank (depends on the wastewater characteristics), and r_ξ is the reaction rate, obtained from the Peterson matrix, using the ASM1 model [10]. There are 13 components in the ASM1 model, however only 11 are considered since two of them are inerts, and they are considered as state variables to the problem: Soluble substrate (S_S), slowly biodegradable substrate (X_S), heterotrophic active biomass (X_{BH}), autotrophic active biomass (X_{BA}), particulate products arising from biomass decay (X_P), nitrate and nitrite nitrogen (S_{NO}), $NH_4^+ + NH_3$ nitrogen (S_{NH}), soluble biodegradable organic nitrogen (S_{ND}), particulate biodegradable organic nitrogen (X_{ND}), alkalinity (S_{alk}), and dissolved oxygen (S_O) that is the control variable. There are also 8 rate processes: aerobic growth of heterotrophs, anoxic growth of heterotrophs, aerobic growth of autotrophs, decay of heterotrophs, decay of autotrophs, ammonification of soluble organic nitrogen, hydrolysis of entrapped organics and hydrolysis of entrapped organic nitrogen.

The process rates are the following.

Aerobic growth of heterotrophs

$$\rho_1 = \mu_H \left(\frac{S_S}{K_S + S_S}\right)\left(\frac{S_O}{K_{OH} + S_O}\right) X_{BH} \tag{2}$$

Anoxic growth of heterotrophs

$$\rho_2 = \mu_H \left(\frac{S_S}{K_S + S_S}\right)\left(\frac{K_{OH}}{K_{OH} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\eta_g X_{BH} \tag{3}$$

Aerobic growth of autotrophs

$$\rho_3 = \mu_A \left(\frac{S_{NH}}{K_{NH} + S_{NH}}\right)\left(\frac{S_O}{K_{OA} + S_O}\right) X_{BA} \tag{4}$$

Decay of heterotrophs

$$\rho_4 = b_H X_{BH} \tag{5}$$

Decay of autotrophs

$$\rho_5 = b_A X_{BA} \tag{6}$$

Ammonification of soluble organic nitrogen

$$\rho_6 = k_a S_{ND} X_{BH} \tag{7}$$

Hydrolysis of entrapped organics

$$\rho_7 = k_h \frac{\frac{X_S}{X_{BH}}}{K_X + \frac{X_S}{X_{BH}}}\left[\left(\frac{S_O}{K_{OH+S_O}}\right) + \eta_h \left(\frac{K_{OH}}{K_{OH} + S_O}\right)\left(\frac{S_{NO}}{K_{NO} + S_{NO}}\right)\right] X_{BH} \tag{8}$$

Hydrolysis of entrapped organic nitrogen

$$\rho_8 = \rho_7 \frac{X_{ND}}{X_S} \tag{9}$$

X denotes the suspended compounds (X_S, X_I, X_{BH}, X_{BA}, X_P) and S the dissolved compounds (S_O, S_S, S_{NO}, S_{NH}, S_{ND}, S_{alk}). The subscripts inf, in, r and ef stands for influent, entry of the tank, recycle and effluent (see Figure 1). The mass balances for the inert materials, S_I and X_I, are not considered because they are transport-only components.

Soluble substrate (S_S)

$$\frac{dS_S}{dt} = \frac{Q}{V_a}\left(S_{S_{in}} - S_S\right) - \frac{1}{Y_H}\rho_1 - \frac{1}{Y_H}\rho_2 + \rho_7; \tag{10}$$

Slowly biodegradable substrate (X_S)

$$\frac{dX_S}{dt} = \frac{Q}{V_a}\left(X_{S_{in}} - X_S\right) + (1 - f_P)\rho_4 + (1 - f_P)\rho_5 - \rho_7; \tag{11}$$

Heterotrophic active biomass (X_{BH})

$$\frac{dX_{BH}}{dt} = \frac{Q}{V_a}\left(X_{BH_{in}} - X_{BH}\right) + \rho_1 + \rho_2 - \rho_4; \tag{12}$$

Autotrophic active biomass (X_{BA})

$$\frac{dX_{BA}}{dt} = \frac{Q}{V_a}\left(X_{BA_{in}} - X_{BA}\right) + \rho_3 - \rho_5; \tag{13}$$

Particulate products arising from biomass decay (X_P)

$$\frac{dX_P}{dt} = \frac{Q}{V_a}\left(X_{P_{in}} - X_P\right) + f_P\rho_4 + f_P\rho_5; \tag{14}$$

Nitrate and nitrite nitrogen (S_{NO})

$$\frac{dS_{NO}}{dt} = \frac{Q}{V_a}\left(S_{NO_{in}} - S_{NO}\right) - \frac{1 - Y_H}{2.86 Y_H}\rho_2 + \frac{1}{Y_A}\rho_3; \tag{15}$$

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

$$\frac{dS_{NH}}{dt} = \frac{Q}{V_a}\left(S_{NH_{in}} - S_{NH}\right) - i_{X_B}\rho_1 - i_{X_B}\rho_2 - \left(i_{X_B} + \frac{1}{Y_A}\right)\rho_3 + \rho_6; \tag{16}$$

Soluble biodegradable organic nitrogen (S_{ND})

$$\frac{dS_{ND}}{dt} = \frac{Q}{V_a}\left(S_{ND_{in}} - S_{ND}\right) - \rho_6 + \rho_8; \tag{17}$$

Particulate biodegradable organic nitrogen (X_{ND})

$$\frac{dX_{ND}}{dt} = \frac{Q}{V_a}\left(X_{ND_{in}} - X_{ND}\right) + \left(i_{X_B} - f_P i_{X_P}\right)\rho_4 + \left(i_{X_B} - f_P i_{X_P}\right)\rho_5 - \rho_8; \tag{18}$$

Alkalinity (S_{alk})

$$\frac{dS_{alk}}{dt} = \frac{Q}{V_a}\left(S_{alk_{in}} - S_{alk}\right) - \frac{i_{X_B}}{14}\rho_1 + \left(\frac{1-Y_H}{14 \times 2.86 Y_H} - \frac{i_{X_B}}{14}\right)\rho_2 - \left(\frac{i_{X_B}}{14} + \frac{1}{7Y_A}\right)\rho_3 + \frac{1}{14}\rho_6; \tag{19}$$

where Y_A, Y_H, f_P, i_{X_B} and i_{X_P} are stoichiometric parameters.

Oxygen (S_O)

$$\frac{dS_O}{dt} = \frac{Q}{V_a}\left(S_{O_{in}} - S_O\right) + K_L a\left(S_{O_{sat}} - S_O\right) - \frac{1-Y_H}{Y_H}\rho_1 - \frac{4.57 - Y_A}{Y_A}\rho_3, \tag{20}$$

where $K_L a$ is the overall mass transfer coefficient.

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

$$K_L a = \frac{\alpha\ G_S\ \eta\ P_{O_2}\ 1333.3}{V_a S_{O_{sat}}}\theta^{(T-20)} \tag{21}$$

where

$$S_{O_{sat}} = \frac{1777.8\beta\rho P_{O_2}}{Henry O_2}, \tag{22}$$

$$\rho = 999.96(2.29 \times 10^{-2}T) - (5.44 \times 10^{-3}T^2),\ Henry O_2 = 708\ T + 25700, \tag{23}$$

and G_S is the air flow rate and α, β, ρ, η, P_{O_2}, T, and θ are operational parameters.

These balances are the first set of ordinary differential equation constraints to the problem, and are discretized using first order Euler's method:

$$\xi_{i+1} = \xi_i + h\left[\frac{Q}{V_a}(\xi_{in} - \xi_i) + r_{\xi_i},\right] \tag{24}$$

where h is the discretization step.

To maintain the system consistence, suspended and dissolved matter balances are included. There are 7 and 6 constraints, respectively, along 24 hours operation.

$$\begin{aligned}(1+r)Q_{inf}TSS_{in} &= Q_{inf}TSS_{inf} + (1+r)Q_{inf}TSS \\ &\quad - \frac{V_a TSS}{SRT\, X_r}(SSI - SSI_{ef}) - Q_{inf}SSI_{ef}\end{aligned} \tag{25}$$

$$\begin{aligned}(1+r)Q_{inf}X_{S_{in}} &= Q_{inf}X_{S_{inf}} + (1+r)Q_{inf}X_S \\ &- \frac{V_aX}{SRTX_r}(X_{S_r} - X_{S_{ef}}) - Q_{inf}X_{S_{ef}}\end{aligned} \tag{26}$$

$$\begin{aligned}(1+r)Q_{inf}X_{I_{in}} &= Q_{inf}X_{I_{inf}} + (1+r)Q_{inf}X_I \\ &- \frac{V_aX}{SRTX_r}(X_{I_r} - X_{I_{ef}}) - Q_{inf}X_{I_{ef}}\end{aligned} \tag{27}$$

$$\begin{aligned}(1+r)Q_{inf}X_{BH_{in}} &= Q_{inf}X_{BH_{inf}} + (1+r)Q_{inf}X_{BH} \\ &- \frac{V_aX}{SRTX_r}(X_{BH_r} - X_{BH_{ef}}) - Q_{inf}X_{BH_{ef}}\end{aligned} \tag{28}$$

$$\begin{aligned}(1+r)Q_{inf}X_{BA_{in}} &= Q_{inf}X_{BA_{inf}} + (1+r)Q_{inf}X_{BA} \\ &- \frac{V_aX}{SRTX_r}(X_{BA_r} - X_{BA_{ef}}) - Q_{inf}X_{BA_{ef}}\end{aligned} \tag{29}$$

$$\begin{aligned}(1+r)Q_{inf}X_{P_{in}} &= Q_{inf}X_{P_{inf}} + (1+r)Q_{inf}X_P \\ &- \frac{V_aX}{SRTX_r}(X_{P_r} - X_{P_{ef}}) - Q_{inf}X_{P_{ef}}\end{aligned} \tag{30}$$

$$\begin{aligned}(1+r)Q_{inf}X_{ND_{in}} &= Q_{inf}X_{ND_{inf}} + (1+r)Q_{inf}X_{ND} \\ &- \frac{V_aX}{SRTX_r}(X_{ND_r} - X_{ND_{ef}}) - Q_{inf}X_{ND_{ef}}\end{aligned} \tag{31}$$

$$(1+r)Q_{inf}S_{S_{in}} = Q_{inf}S_{S_{inf}} + rQ_{inf}S_{S_r} \tag{32}$$

$$(1+r)Q_{inf}S_{O_{in}} = Q_{inf}S_{O_{inf}} + rQ_{inf}S_{O_r} \tag{33}$$

$$(1+r)Q_{inf}S_{NO_{in}} = Q_{inf}S_{NO_{inf}} + rQ_{inf}S_{NO_r} \tag{34}$$

$$(1+r)Q_{inf}S_{NH_{in}} = Q_{inf}S_{NH_{inf}} + rQ_{inf}S_{NH_r} \tag{35}$$

$$(1+r)Q_{inf}S_{ND_{in}} = Q_{inf}S_{ND_{inf}} + rQ_{inf}S_{ND_r} \tag{36}$$

$$(1+r)Q_{inf}S_{alk_{in}} = Q_{inf}S_{alk_{inf}} + rQ_{inf}S_{alk_r} \tag{37}$$

being $X = X_I + X_S + X_{BH} + X_{BA} + X_P$.
SRT is the sludge retention time and is given by

$$SRT = \frac{V_aX}{Q_wX_r}, \tag{38}$$

HRT is the hydraulic retention time and is given by

$$HRT = \frac{v_a}{Q}, \tag{39}$$

and r is the recycle rate and is given by

$$r = \frac{Q_r}{Q_{inf}}. \tag{40}$$

The flow balances also have to be included, according to the points showed in Figure 1, to maintain the system cohesive. The flows in each part of the system are also considered as state variables. This gives rise to a set of 3 constraints, also solved in the 24 hours operation considered in the problem.

$$Q_r = rQ_{inf} \tag{41}$$

$$Q = Q_{inf} + Q_r \tag{42}$$

$$Q = Q_{ef} + Q_r + Q_w \tag{43}$$

The last set of equations comprise the Portuguese law limits, in terms of Chemical Oxygen Demand (COD), Total Suspended Solids (TSS) and Total Nitrogen (N). These composite variables are measured as a composition of the state variables defined in the first set of constraints as

$$COD = X_I + X_S + X_{BH} + X_{BA} + X_P + S_I + S_S \tag{44}$$

$$TSS = \frac{X_I + X_S + X_{BH} + X_{BA} + X_P}{icv} + ISS \tag{45}$$

$$N = S_{NH} + S_{ND} + X_{ND} + i_{X_B}(X_{BH} + X_{BA}) i_{X_P}(X_P + X_I) - S_{NO} \tag{46}$$

There are also 3 inequality constraints along the 24 hours operation.

$$COD_{ef} \leq COD_{law} \tag{47}$$

$$N_{ef} \leq N_{law} \tag{48}$$

$$TSS_{eef} \leq TSS_{law} \tag{49}$$

All variables must be non-negative, but due to operational constraints some more restricted bounds are imposed as follows:

$$\begin{aligned} 0 \leq & K_{LA} \leq 300, \\ 0.05 \leq & HRT \leq 2, \\ 800 \leq & TSS \leq 6000, \\ 0.5 \leq & r \leq 2, \\ 2500 \leq & TSS_r \leq 10000, \\ 6 \leq & S_{alk} \leq 8, \\ 6 \leq & S_{alk_{in}} \leq 8, \\ 2 \leq & S_O \leq 5 \end{aligned} \tag{50}$$

In this work, an optimal control approach is conducted in order to simulate distinct features of a mathematical model.

3. **Optimal control problem.** Due to population growth and consequent increase in the amount of wastewater generated, it is expected that the consumption of energy due to oxygen consumption by the bacteria grows. However, the requirements in terms of the quality of the wastewater will be increasingly restrictive. All stages of the treatment process must be controlled and managed to improve the quality of the final effluent, reducing its environmental impact. This way, it is necessary to have a tradeoff between the cost associated with increasing the levels of dissolved oxygen and the costs of having a good quality index in the effluent.

An optimal control problem is formulated as follows.

$$\min_{\Omega} J(u(\cdot)) = \int_0^{T_f} \left[\omega_1 u(t) + \omega_2 QI(t)\right] \, dt, \tag{51}$$

subject to all the constraints defined in Section 2.
The control variable u is the S_O and $\omega_i > 0$, $i = 1, 2$, are the weights of the investment costs associated to the control variable, S_O and the state variable, QI, respectively ($\sum_{i=1}^{2} \omega_i = 1$). There exists a trade-off between oxigen dissolved (S_O) and quality index (QI) - if the goal is to give more relevance to S_O then ω_1 should be increased (economist perspective, saving money), for other hand, ω_2 should be increased if the main concern is to improve the quality index (QI) (environmental perspective).

To solve the problem (51) two different strategies can be considered: indirect and direct methods. Indirect methods are based on the Pontryagin's Maximum Principle (PMP) [14] to compute the optimal solution. On the other hand, direct methods discretize all the variables (state and control) with respect to time, in which the cost functional is directly optimized, considering the optimal control problem as a nonlinear optimization problem (NLP) [2]. Some advantages and drawbacks can be pointed out to both methods: direct methods are more easier to implement, more robust and less sensitive to the initial conditions than indirect methods. However, indirect methods provide high levels of numerical accuracy but their implementation is more difficult needing to compute the derivatives and the necessary conditions related to PMP [18].

The problem presented was solved by direct methods. A direct method is iterative, constructing a sequence of points $x_1, x_2, \dots, x^*$ such that the objective function is minimized and typical $F(x_1) > F(x_2) > \dots > F(x^*)$. The approximation to the solution in iteration i is denoted by x_i. The optimal solution of (51) is x^* and $F(x)$ is the objective function of (51) to be minimized. Here the state and/or control are approximated using an appropriate function approximation (e.g., polynomial approximation or piecewise constant parameterization). Simultaneously, the cost functional is approximated as a cost function. Then, the coefficients of the function approximations are treated as optimization variables and the problem is reformulated to a standard nonlinear optimization problem (NLP). In fact, the NLP is easier to solve than the boundary-value problem, mainly due to the sparsity of the NLP and the many well-known software programs that can handle with this feature. As a result, the range of problems that can be solved via direct methods is significantly larger than the range of problems that can be solved via indirect methods (see page 19 of [17]).

4. **Methodology.** The formulated NLP is solved using Ipopt [20] via NEOS server platform [5]. The `Ipopt`, *Interior Point OPTimizer*, is a software package for large-scale nonlinear optimization. It is written in `Fortran` and `C`. `Ipopt` implements a primal-dual interior point method and uses a line search strategy based on filter method. `Ipopt` can be used from various modeling environments. `Ipopt` is designed to exploit 1st and 2nd derivative information if provided, usually via automatic differentiation routines in modeling environments such as `AMPL`. If no Hessians are provided, `Ipopt` will approximate them using a quasi-Newton methods, specifically a BFGS update [17].

In NEOS platform there is a large set of optimization software packages. NEOS is considered as the state of the art in optimization and includes the `Ipopt`. The programming language used was AMPL [8]. This way the model organizes and automates the tasks of modelling, which can handle a large volume of data and, moreover, can be used in machines and independent solvers, allowing the user to concentrate on the model instead of the methodology to reach solution.

However, the `AMPL` modelling language itself does not allow the formulation of differential equations being necessary to discretize the problem. Therefore, for this problem, the discretization process selected was the Euler scheme. Previous experiences by the authors for other optimal control problems, showed that the effort of the implementation of higher order discretization methods, like Runge-Kutta, brings no advantages to the solution [16].

In the discretization procedure we use an one hour step, during 24 hours ($T_f = 24$). The NLP problem was coded in the AMPL mathematical modeling language [8] and has 1031 variables (958 nonlinear and 73 linear), 710 constraints (566 nonlinear, 144 linear), being 638 equality constraints and 72 inequality constraints.

4.1. **Parameters and initial values.** The optimal control problem is solved by finding the optimal dissolved oxygen concentration in the aeration tank, and the optimal quality index, during one day (24 hours) of operation of an activated sludge tank (51), respecting all the problem constraints (10) to (50).

We considered a typical domestic effluent entering the WWTP, with a constant composition during an operation day. It was considered the Portuguese law limits in terms of COD, TSS and N (125 g/m^3, 35 g/m^3 and 15 g/m^3, respectively).

Table 1 lists all the variables involved, as well as the considered initial values provided to the solver.

Table 2 shows the parameters values, and Table 3 lists the characteristics of the wastewater entering the system. These are typical values found in a domestic wastewater and in the operation of an activated sludge system, and they were obtained from [6].

5. **Computational results.** The simulations for this NPL problem were conducted having two main purposes in mind: to understand the influence of initial pollution S_{inf} when arrives to the plant (Section 5.1), and to study the impact of distinct weighs in the optimal control function (Section 5.2). The results from `Ipopt` are compiled in Matlab graphics.

5.1. **The influence of S_{inf} in the model.** In order to understand the impact of the level of polluted wastewater arriving to the plant, different experiences were made for distinct values of S_{inf}. These experiences also considered different values

TABLE 1. Variables of the problem and initial values

Variable	Init.val.	Variable	Init.val.	Variable	Init.val.
Q	4000	Q_w	100	Q_r	2000
Q_{ef}	1900	X_I	727.3	X_{I_r}	950.571
$X_{I_{ef}}$	10^{-5}	$S_{S_{in}}$	50	S_S	10
$S_{O_{in}}$	1	$S_{NO_{in}}$	10^{-6}	S_{NO}	10^{-6}
$X_{BH_{in}}$	0.2	X_{BH}	350	X_{BH_r}	711.2
$X_{BH_{ef}}$	10^{-5}	$X_{S_{in}}$	3000	X_S	350
X_{S_r}	806.714	$X_{S_{ef}}$	10^{-5}	$X_{BA_{in}}$	10^{-5}
X_{BA}	10^{-6}	X_{BA_r}	1.9×10^{-6}	$X_{BA_{ef}}$	10^{-5}
$S_{NH_{in}}$	10	S_{NH}	7.5	$X_{P_{in}}$	1500
X_P	90	X_{P_r}	174.52	$X_{P_{ef}}$	10^{-5}
$S_{ND_{in}}$	0.5	S_{ND}	0.5	$X_{ND_{in}}$	200
X_{ND}	20	X_{ND_r}	20	$X_{ND_{ef}}$	0.5
G_S	10000	SSI	1500	SSI_{ef}	0.1
SSI_r	3500	HRT	3.5	r	1
S_O	2				

TABLE 2. Parameters

Kinetic		Operational		Stoichiometric	
μ_H	6	T	20	Y_A	0.24
μ_A	0.8	P_{O_2}	0.21	Y_H	0.666
k_h	3	SRT	20	f_P	0.08
k_a	0.08	θ	1.024	i_{X_B}	0.086
b_h	0.62	α	0.8	i_{X_P}	0.06
b_a	0.04	η	0.07		
η_g	0.8	β	0.95		
η_h	0.4				
K_S	20				
K_X	0.03				
K_{OH}	0.2				
K_{NO}	0.5				
K_{NH}	1				
K_{OA}	0.4				

for the weights related to the variables inclued in the optimal control function: $(\omega_1, \omega_2) = (1, 0)$, $(\omega_1, \omega_2) = (0.5, 0.5)$ and $(\omega_1, \omega_2) = (0, 1)$ in (51).

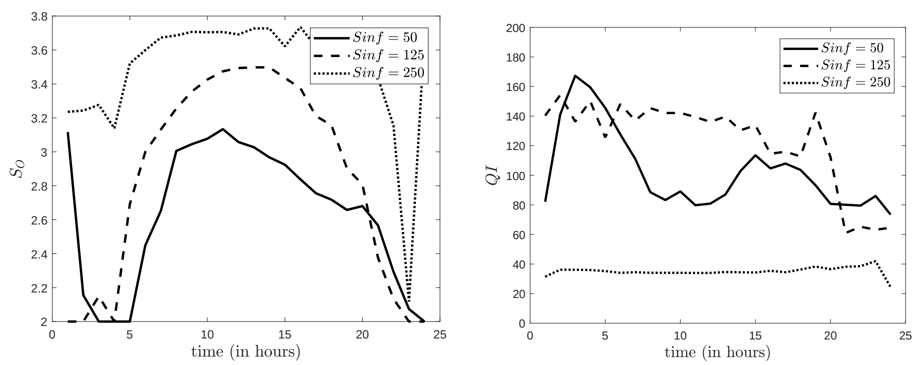
Figures 2, 3 and 4, and Table 4 present the results for three scenarios (A, B and C), where the weighs ω_1 and ω_2 varies.

According to Figures 2, 3 and 4 the results have physical meaning, since the dissolved oxygen is always above the required minimum of 2 mg/L (Figures 2(a), 3(a) and 4(a)). Also, the law limits are always accomplished since the solution is always feasible. It can be observed that, in general, the effluent quality trends to deteriorate when the amount of oxygen is lower (Figures 2(b), 3(b) and 4(b)). As expected, the more polluted the wastewater is, the more oxygen is demanded.

Table 4 shows the total amount of S_O and QI considering differents amounts of pollution S_{inf}. In Scenario A, an economist vision with $(\omega_1, \omega_2) = (1, 0)$, the aim is

TABLE 3. Characteristics of the wastewater entering the system

Q_{inf}	530
$S_{I_{inf}}$	5.45, 12.5 and 25
S_S	44.55, 112.5 and 225
S_{inf}	50, 125 and 250
$X_{BH_{inf}}$	0
$X_{BA_{inf}}$	0
$X_{P_{inf}}$	0
$S_{O_{inf}}$	0
$S_{NO_{inf}}$	0
$S_{alk_{inf}}$	7
$X_{I_{inf}}$	90
$X_{S_{inf}}$	168.75
$S_{NH_{inf}}$	11.7
$X_{S_{inf}}$	168.75
$S_{NH_{inf}}$	11.7
$S_{ND_{inf}}$	0.63
$X_{ND_{inf}}$	1.251
X_{II}	18.3



(a) Dissolved oxygen (control).

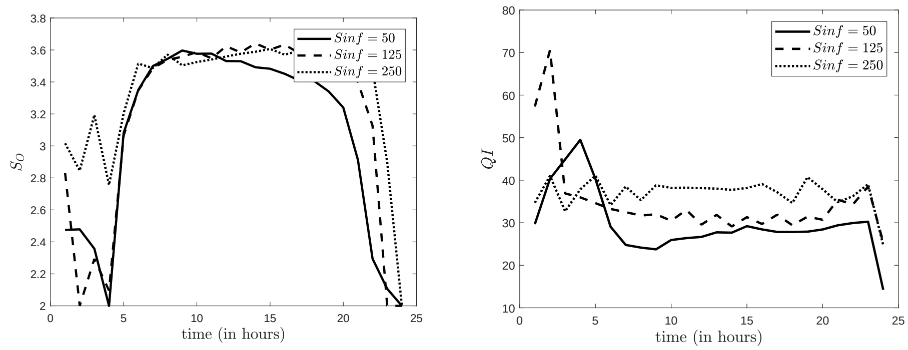
(b) Quality index.

FIGURE 2. Hourly results during one day with $(\omega_1, \omega_2) = (1, 0)$.

TABLE 4. Results for three different amounts of pollution in the wastewater

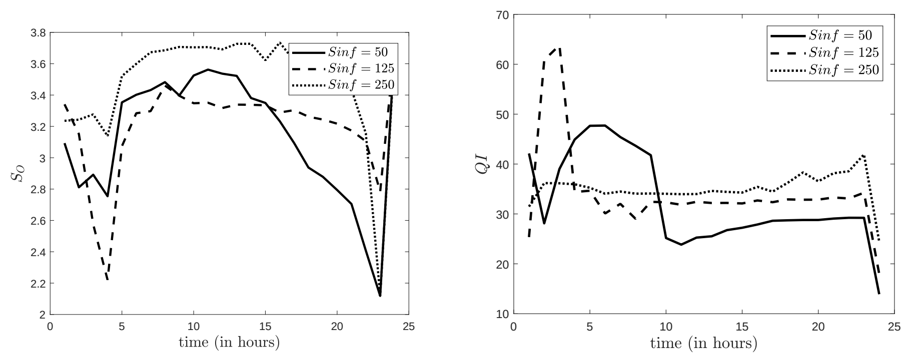
	Scenario A $(w_1, w_2) = (1, 0)$			Scenario B $(w_1, w_2) = (0.5, 0.5)$			Scenario C $(w_1, w_2) = (0, 1)$		
S_{inf}	50	125	250	50	125	250	50	125	250
S_O	60.6	66.4	80.2	71.5	73.8	77.9	72.0	73.4	80.2
QI	2390.6	2849.9	813.1	692.3	795.4	857.2	750.2	750.4	813.1

only to minimize the demanded oxygen (the cost), and there is not a direct impact in the quality index as the systems progresses only to maintain the dissolved oxygen to accomplish the demanded quality.



(a) Dissolved oxygen (control). (b) Quality index.

FIGURE 3. Hourly results during one day with $(\omega_1, \omega_2) = (0.5, 0.5)$.



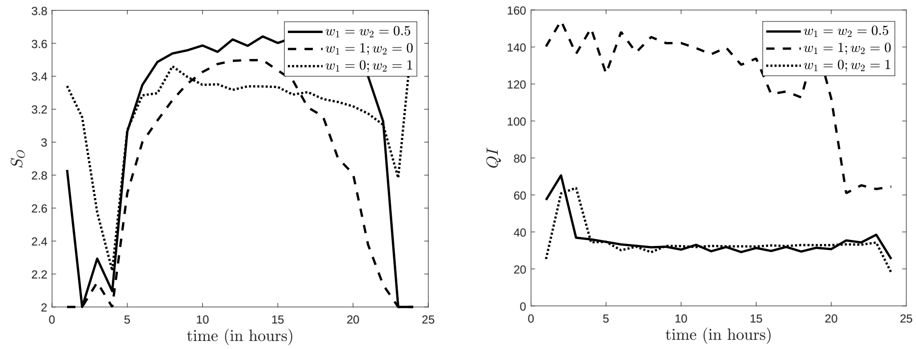
(a) Dissolved oxygen (control). (b) Quality index.

FIGURE 4. Hourly results during one day with $(\omega_1, \omega_2) = (0, 1)$.

In Scenario C with $(\omega_1, \omega_2) = (0, 1)$, a more environmental perspective, the aim is to minimize the amount of pollution in the effluent, regardless the cost. In this scenario the quality deteriorates when the wastewater at the entry is more polluted and the oxygen level only rises slightly, being more independent of the wastewater characteristics in this case.

Finally, in Scenario B, $(\omega_1, \omega_2) = (0.5, 0.5)$, it is a balanced scenario, and a trade-off is performed between both goals. Like in Scenario A, while the total oxygen demanded during one day is bigger as the wastewater is more polluted, the amount of pollution is more independent in relation to the quality of the wastewater. This means that the system can give a response when controlling the dissolved oxygen, being able to tackle a more polluted water.

5.2. **The influence of w_1 and w_2 in the model.** To better assessment of the results above, we set $S_{inf} = 125$ and the results can be seen in Figure 5. From an economist point of view, when $(w_1, w_2) = (1, 0)$ the figure shows that when the



(a) Dissolved oxygen (control).

(b) Quality index.

FIGURE 5. Hourly results during one day with $S_{inf} = 125$.

only goal is to save money – meaning to use the minimal quantity of oxygen – the quality index worsens throughout the day.

In this scenario A the limit in TSS_{ef} is reached throughout almost the entire day (Figure 6(b)) and the N_{ef} presented the higher values (Figure 6(c)). In scenario C, $(\omega_1, \omega_2) = (0, 1)$, it was observed that the limit in COD_{ef} is reached at the beginning of the day (Figure 6(a)).

The environmental perspective (Scenario C), as expected, whose only goal is to optimize the quality index, presents the higher total value of the dissolved oxygen, resulting in a much expensive solution. The Scenario B takes into account both goals presenting intermediate values for the control variable S_O and the state variable QI, being the bioeconomic perspective.

6. **Conclusions and Future directions.**

Water has been one of the essential factors in the development of human settlements. The increasing population of human and industry, lead to the increasing of water demand, as well as more and more polluted wastewater. So, the treatment of wastewater rapidly became a primordial importance subject. With the wastewater treatment expensive processes arises.

The discussed results demonstrated that the control of the dissolved oxygen – the variable that most influences the cost and quality of the treated effluent in the activated sludge system herein considered – is crucial. In the scenario that considers no economical concern (Scenario C from Table 4), the dissolved oxygen raises, leading to a higher demand on the oxygen consumption. When the bioeconomic approach is taken into account (Scenario B from Table 4), a more equilibrated solution is found.

This research brings some contributions to both academy and companies. Although this is a theoretical approach, it is not difficult to implement in a real WWTP in operation and to reinforce the results through real simulations. The basis for a diversity of real situations presented in this study, leads to enourmous economic and environmental gains.

Regardless of these potential contributions, it becomes evident that a validation based on real data is mandatory.

As future work, the authors suggest to include different weights in (51) and smaller discretization steps. We also intend to consider a more realistic effluent to the WWTP, since the characteristics of a domestic wastewater varies along the day. Also, a model for the secondary settler should be used to a more realistic solution. Another approaches to be considered is to solve the problem using multiobjective optimization, and indirect methods based on PMP [14]. Besides the dissolved oxygen, other control variables can be used, for instance, the sludge recycle rate, that was set as a parameter in the presented model. The authors also suggest the validation of the results in data from real activated sludge systems in operation.

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REFERENCES

[1] L. Amand and B. Carlsson. Optimal aeration control in a nitrifying activated sludge process. Water Research, vol. 46, no.7, pp. 2101–2110, 2012.

[2] M.S. Bazaraa, H.D. Sherali and C.M. Shetty. Nonlinear programming: theory and algorithms John Wiley & Sons, 2013.

[3] C. Binnie, M. Kimber and G. Smethurst. Basic Water Treatment. *Royal Society of Chemistry*, Cambridge, UK, 2002.

[4] S.Cristea, C.de Prada, D.Sarabia, G.Gutierrez. Aeration control of a wastewater treatment plant using hybrid NMPC. Computers & Chemical Engineering, vol. 35, no. 4, pp. 638–650, 2011.

[5] J. Czyzyk, M.P. Mesnier and J.J. Moré. The NEOS server. IEEE Computational Science and Engineering, vol. 5, no. 3, pp. 68–75, 1998.

[6] I. Esprito Santo, *Desenho ptimo de estaes de guas residuais atravs da modelao dee funes custo*, Ph.D thesis, Universidade do Minho, Braga, 2007.

[7] M. Fikar, B. Chachuat and M.A. Latifi. Optimal operation of alternating activated sludge processes. Control Engineering Practice, vol.13, no. 7, pp. 853–861, 2005.

[8] R. Fourer, D. M. Gay, and B. Kernighan. AMPL: a mathematical programming language. Algorithms and model formulations in mathematical programming, Stein W. Wallace (Ed.). Nato Asi Series F, Computer And Systems Sciences, Vol. 51. Springer-Verlag, Berlin, Heidelberg 150-151, 1989.

[9] G. Fu, D. Butler, S.T. Khu. Multiple objective optimal control of integrated urban wastewater systems. Environmental Modelling & Software, vol. 23, no. 2, pp 225–234, 2008.

[10] M. Henze, C. P. L. Grady Jr, W. Gujer, G. V. R. Marais, and T. Matsuo. "Activated sludge model no. 1," *Technical Report 1, IAWPRC Task Group on Mathematical Modelling for design and operation of biological wastewater treatment*, 1986.

[11] H. W. Hethcote. *The mathematics of infectious diseases* SIAM Rev. 42, pp. 599–653, 2000.

[12] B. Holenda, E. Domokos, Á. Rédey and J. Fazakas. Aeration optimization of a wastewater treatment plant using genetic algorithm. Optimal Control Applications and Methods, vol. 28, no. 3, pp. 191–208, 2007.

[13] R. Hreizab, N. Roche, B. Benyahiac, M.A.Latifia. Multi-objective optimal control of small-size wastewater treatment plants. Chemical Engineering Research and Design, vol. 102, pp. 345–353, 2015.

[14] L.S. Pontryagin. Mathematical theory of optimal processes CRC Press, 1987.

[15] J.F. Qiao, Y. C. Bo ; W. Chai ; H.G. Han. Adaptive optimal control for a wastewater treatment plant based on a data-driven method. Water Science & Technology, vol. 67, no. 10, pp. 2314–2320, 2013.

[16] H. S. Rodrigues, M. T. T. Monteiro, D.F.M. Torres. Optimization of dengue epidemics: a test case with different discretization schemes. AIP Conference Proceedings 1168, pp. 1385-1388, 2009.

[17] H. S. Rodrigues. Optimal Control and Numerical Optimization Applied to Epidemiological Models. *PhD thesis*, University of Aveiro, 2012.

[18] H. S. Rodrigues, M. T. T. Monteiro, D.F.M. Torres. Optimal Control and numerical software: an overview. *In* Systems Theory: perspectives, applications and developments, pp.93-110, 2014.

[19] C. Sweetapple, G. Fu and D. Butler. Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions. Water Research, vol. 55, no. 15, pp. 52–62, 2014.

[20] A. Wätcher and L.T. Biegler. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. Mathematical programming, vol. 106, no. 1, pp. 25–57, 2006.

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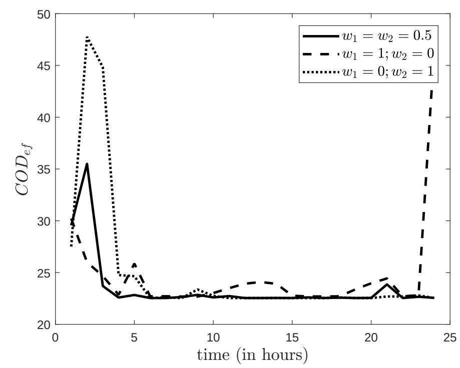
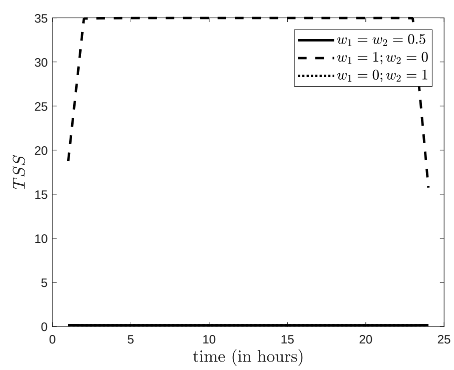
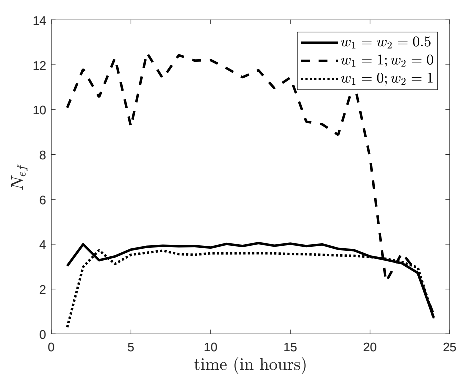


(a) COD at the effluent.



(b) TSS at the effluent.



(c) N at the effluent.

FIGURE 6. Hourly results for the law limits during one day with $S_{inf} = 125$.