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New Optimal Control Problems for Wastewater Treatment with Different Types of Bacteria

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Abstract: The aim of this paper is to propose mathematical models to predict and optimize the cost of wastewater treatment using bacteria and oxygen under fluctuating resource and cultivation conditions. We have thus developed deterministic mathematical models based on dynamic systems and applied optimal control theory to reduce treatment costs. Two wastewater treatment models are proposed: one using only one type of aerobic bacteria, thermophilic bacteria; and the second using two types of aerobic bacteria, thermophilic and mesophilic bacteria. For each model, an optimal control problem is solved and numerical simulations illustrate the theoretical results.

Keywords: wastewater; aerobic bacteria; oxygen; dynamical system; ordinary differential equation; optimal control; Pontryagin's maximum principle

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1. Introduction

Over the past 40 years, water resources have become increasingly significant. This is due to the growth of the global population and the rapid development of industries, causing serious environmental challenges because of the large quantities of wastewater that are released [1–4]. After use, the majority of wastewater is discharged without any pre-treatment, resulting in the degradation of water quality, since the flow of wastewater discharge is too significant for natural regeneration. Many countries have established regulation limits on the discharge rate into the environment. Consequently, wastewater must be treated before being discharged into natural bodies of water. Various processes are employed to reduce the negative impacts on environment and health.

Wastewater treatment processes require several phases, each one addressing a specific type of pollution. The activated sludge treatment phase, whose operating principle is described in [5–9], is the key phase of the treatment chain. This activated sludge treatment process consists of bringing the organic matter in the wastewater into contact with a bacterial population. The bacteria assimilate the organic matter for their own development. This process is called activated sludge treatment because all conditions that maximize bacteria activity are implemented such as sufficient oxygen supply, nutrient addition if the effluent does not contain all the compounds necessary for bacteria development, continuous agitation to promote contact between bacteria and pollutants, and a high concentration of bacteria to increase treatment efficiency. Activated sludge treatment is very effective but energy-intensive, since non-pathogenic bacteria need to be in well-oxygenated water

to assimilate pollutants, and oxygenation consumes a large amount of energy. Different control strategies for the activated sludge process have been carried out to reduce treatment costs [5,9–12].

The contribution of this work is divided into two parts: The first part concerns wastewater treatment with only one type of bacteria, and the second part concerns two types of bacteria. In the second section, we extend a model proposed by Grigorieva et al. in [13], in which we add a substrate production term due to bacterial death. We separately study two optimal control problems: the first one to minimize the concentration of pollutants at the end of treatment, and the second one to minimize the concentration of pollutants throughout treatment. For these problems, the control variable is the oxygen injection rate in the reactor. By applying the Pontryagin maximum principle, we characterize in each case the optimal control, and numerical simulations are then performed to illustrate our theoretical study. In the third section, we extend the model proposed in the second one by considering two types of aerobic bacteria, mesophilic and thermophilic ones, as these are present in the case of wastewater treatment [14]. In this case, we consider an optimal control problem consisting of minimizing the weighted sum of the pollutants' concentrations at the end of the treatment and the operational costs of oxygen pumping, again by controlling the oxygen injection rate. By applying the Pontryagin maximum principle, we characterize the optimal control and numerical simulations are given to illustrate our theoretical study. The techniques and methods used in this paper are almost similar to those of [13] but more complicated due to the addition of terms and equations.

2. Study of Two Optimal Control Problems for a Wastewater Treatment Model with One Type of Bacteria

The mathematical model that we propose is an extension of the one in [13] and can be formulated as a system of three ordinary differential equations:

$$\begin{cases} \dot{x}(t) = -x(t)y(t)z(t) + u(t)(m - x(t)), & t \in [0, T], \\ \dot{y}(t) = -x(t)y(t)z(t) + fz(t), \\ \dot{z}(t) = x(t)y(t)z(t) - \alpha z(t), \\ x(0) = x_0 \in (0, m), \quad y(0) = y_0 > 0, \quad z(0) = z_0 > 0 \end{cases} \quad (1)$$

where $x(\cdot)$ is the concentration of oxygen, $y(\cdot)$ is the concentration of pollutants, $z(\cdot)$ is the concentration of thermophilic aerobic bacteria, $u(\cdot)$ is the oxygen pumping rate, m is the oxygen saturation point in the treatment unit, α is the natural mortality rate of bacteria, f is the fraction of dead bacteria transformed into a new pollutant, and T is the treatment duration. With this model, we assume that the reaction is described by the mass action law introduced in [15], which characterizes the chemical reaction as a function of the concentration of the initial substances. We consider variables without dimensions, as it is usually considered in studies of this type [16,17]. As in [13], each variable is normalized with some limiting value that exists, as we will see in the following Proposition 1. Moreover, for all $t \in [0, T]$, $x(t) < m$, and this will be proven in the following Proposition 1.

The first equation of System (1) describes the evolution of oxygen concentrations in the reactor. The first term describes the oxygen absorption process in the reaction, while the second one is the inflow of oxygen (through pumping) into the reactor from the outside. Dissolved oxygen is replenished by aeration, subject to the saturation concentration m . Here, $u(\cdot)$ is the aeration rate, which will also be the control function in the following. In the second equation, the first term describes a decrease in organic matter in the reaction and the second one is the production of organic matter due to bacterial decomposition, with a recycled fraction f as substrate. The third equation describes the evolution of aerobic

bacteria. The first term describes its growth and the second term describes its reduction due to natural mortality at a rate α with $\alpha > f$. It is important to notice that this model (1) is different from the one in [13] due to the addition of the term $fz(\cdot)$ representing the formation of new pollutants as the substrate. Indeed, in the model proposed by Grigorieva et al. in [13], the term $fz(\cdot)$ does not exist. The addition of this term is justified by the fact that the natural death of the bacteria leads to the production of a certain amount of pollutants, which also justifies the choice of the hypothesis $f < \alpha$.

Moreover, the set of admissible controls, denoted by $\mathcal{U}$, is the set of all Lebesgue measurable functions $u(t)$ such that, for almost every $t \in [0, T]$,

$$0 \leq u(t) \leq u_{\max}, \quad (2)$$

where $u_{\max}$ is the maximum aeration rate. Our goal is to separately solve the two following optimal control problems:

$$(\mathcal{P}) \quad J(u) = y(T) \longrightarrow \min_{u \in \mathcal{U}} \quad (3)$$

and

$$(\tilde{\mathcal{P}}) \quad \tilde{J}(u) = \int_0^T y(t) dt \longrightarrow \min_{u \in \mathcal{U}}. \quad (4)$$

Proposition 1. For all control $u(\cdot) \in \mathcal{U}$, all trajectories $x(\cdot)$, $y(\cdot)$, and $z(\cdot)$ of (1), starting in the positive orthant, are bounded and, for all $t \geq 0$,

$$0 < x(t) < m, \quad 0 < y(t) < y_{\max}, \quad 0 < z(t) < z_{\max}, \quad (5)$$

where $y_{\max} = y_0 + fz_{\max}T$ and $z_{\max} = x_0 + z_0 + mu_{\max}T$.

Proof. By using the third equation of System (1), we get

$$z(t) = z_0 \exp\left(\int_0^t (x(\epsilon)y(\epsilon) - \alpha)d\epsilon\right). \quad (6)$$

It follows that, for all $t \geq 0$, $z(t) > 0$. Next, using the second equation of System (1), we get

$$y(t) = \exp\left(-\int_0^t x(\epsilon)z(\epsilon)d\epsilon\right)\left(y_0 + f\int_0^t \exp\left(\int_0^s (x(\epsilon)z(\epsilon)d\epsilon\right)z(s)ds\right). \quad (7)$$

Hence, for all $t \geq 0$, $y(t) > 0$. Finally, with the first equation of System (1), we have

$$x(t) = \exp\left(-\int_0^t (y(\epsilon)z(\epsilon) + u(\epsilon))d\epsilon\right)\left(x_0 + m\int_0^t \exp\left(\int_0^s (y(\epsilon)z(\epsilon) + u(\epsilon))d\epsilon\right)u(s)ds\right).$$

Consequently, $x(t) > 0$ for all $t \geq 0$. Let us now prove that these solutions are bounded. First, we show that $x(t) < m$, for all $t \geq 0$. For this, we consider the function $\gamma(t) = m - x(t)$ and use the first equation of System (1) to obtain that γ is the solution to the Cauchy problem:

$$\begin{cases} \dot{\gamma}(t) = -(y(t)z(t) + u(t))\gamma(t) + my(t)z(t) \\ \gamma(0) = \gamma_0 = m - x_0 > 0. \end{cases} \quad (8)$$

We remark that γ could be expressed by

$$\gamma(t) = \exp\left(-\int_0^t (y(\epsilon)z(\epsilon) + u(\epsilon))d\epsilon\right)\left(\gamma_0 + m\int_0^t \exp\left(\int_0^s (y(\epsilon)z(\epsilon) + u(\epsilon))d\epsilon\right)y(s)z(s)ds\right),$$

and it is easy to see that for all $t \geq 0$, $\gamma(t) > 0$, which implies that $x(t) < m$, for all $t \geq 0$. Then, adding the first and the third equations of System (1), we get

$$\dot{x}(t) + \dot{z}(t) = -\alpha z(t) + u(t)(m - x(t)), \quad (9)$$

which is equivalent to

$$x(t) + z(t) = x_0 + z_0 - \alpha \int_0^t z(\epsilon) d\epsilon + \int_0^t u(\epsilon)(m - x(\epsilon)) d\epsilon,$$

and implies that

$$x(t) + z(t) < x_0 + z_0 + m \int_0^t u(\epsilon) d\epsilon.$$

Using Inequality (2), we find that $x(t) + z(t) < x_0 + z_0 + mu_{\max}T = z_{\max}$, for all $t \in [0, T]$, which implies that $z(t) < z_{\max}$, for all $t \in [0, T]$. Finally, from (7), we get

$$y(t) = y_0 \exp\left(-\int_0^t x(\epsilon)z(\epsilon) d\epsilon\right) + f \int_0^t \exp\left(-\int_s^t x(\epsilon)z(\epsilon) d\epsilon\right) z(s) ds.$$

Then, $y(t) < y_0 + f \int_0^t z(s) ds$ implies that $y(t) < y_0 + fz_{\max}T = y_{\max}$, for all $t \in [0, T]$. $\square$

Proposition 2. *The two optimal control problems (3) and (4) are well posed in the sense that for each control $u \in \mathcal{U}$, there is one and only one solution to the Cauchy problem (1).*

Proof. For all $u \in \mathcal{U}$, we define the function F by $F(t, X(t)) = f(t, X(t), u(t))$ with

$$X(t) = (x(t), y(t), z(t))^T,$$

$$f(t, X(t), u(t)) = (f_1(t, X(t), u(t)), f_2(t, X(t), u(t)), f_3(t, X(t), u(t)))^T$$

and

$$\begin{cases} f_1(t, X(t), u(t)) = -x(t)y(t)z(t) + u(t)(m - x(t)), \\ f_2(t, X(t), u(t)) = -x(t)y(t)z(t) + fz(t), \\ f_3(t, X(t), u(t)) = x(t)y(t)z(t) - \alpha z(t). \end{cases}$$

It is clear that F is measurable, integrable with respect to t , continuous and locally Lipschitzian with respect to X . Consequently, the Cauchy problem (1) has a unique maximal solution. $\square$

Theorem 1. *The optimal control problem (3) (respectively, (4)) admits an optimal control $u^* \in \mathcal{U}$ (respectively, $\tilde{u}^* \in \mathcal{U}$) such that the associated trajectory (x^*, y^*, z^*) (respectively, $(\tilde{x}^*, \tilde{y}^*, \tilde{z}^*)$) is a solution of the dynamical System (1).*

Proof. It is a consequence of the two previous propositions and the fact that the right-hand sides of the equations of System (1) are convex with respect to u . $\square$

2.1. Study of the Optimal Control Problem ($\mathcal{P}$)

In this section, we will characterize the optimal control u^* associated with problem ($\mathcal{P}$).

By applying the Pontryagin maximum principle [18] for the control $u^*(t)$ and the corresponding solution $X^*(t)$, there exists a non-trivial solution $\psi^*(t) = (\psi_1^*(t), \psi_2^*(t), \psi_3^*(t))$ of the adjoint system:

$$\begin{cases} \dot{\psi}_1^*(t) = u^*(t)\psi_1^*(t) + y^*(t)z^*(t)(\psi_1^*(t) + \psi_2^*(t) - \psi_3^*(t)) \\ \dot{\psi}_2^*(t) = x^*(t)z^*(t)(\psi_1^*(t) + \psi_2^*(t) - \psi_3^*(t)) \\ \dot{\psi}_3^*(t) = x^*(t)y^*(t)(\psi_1^*(t) + \psi_2^*(t) - \psi_3^*(t)) + \alpha\psi_3^*(t) - f\psi_2^*(t) \\ \psi_1^*(T) = 0, \psi_2^*(T) = -1, \psi_3^*(T) = 0, \end{cases} \quad (10)$$

such that the control $u^*(t)$ maximizes the Hamiltonian $\mathcal{H}$ defined by

$$\mathcal{H}(x, y, z, \psi_1, \psi_2, \psi_3, u) = (-xyz + u(m - x))\psi_1 + (-xyz + fz)\psi_2 + (xyz - \alpha z)\psi_3.$$

But $0 \leq u^*(t) \leq u_{max}$, for almost all $t \in [0, T]$, so

$$u^*(t) = \begin{cases} u_{max} & \text{if } L(t) > 0, \\ u^* \in [0, u_{max}] & \text{if } L(t) = 0, \\ 0 & \text{if } L(t) < 0, \end{cases} \quad (11)$$

where $L(t) = \psi_1^*(t)$ is the switching function of problem $(\mathcal{P})$.

In order to study the behaviour of the switching function $L(\cdot)$, we introduce the following auxiliary functions:

$$G(t) = \psi_1^*(t) + \psi_2^*(t) - \psi_3^*(t) \text{ and } P(t) = -\psi_3^*(t) + \alpha^{-1}f\psi_2^*(t).$$

The adjoint System (10) associated with problem $(\mathcal{P})$ can be rewritten with the functions $L(\cdot)$, $G(\cdot)$, and $P(\cdot)$ as

$$\begin{cases} \dot{L}(t) = u^*(t)L(t) + y^*(t)z^*(t)G(t) \\ \dot{G}(t) = u^*(t)L(t) + h(t)G(t) + \alpha P(t) \\ \dot{P}(t) = \rho(t)G(t) + \alpha P(t) \\ L(T) = 0, G(T) = -1, P(T) = -\alpha^{-1}f, \end{cases} \quad (12)$$

where $\rho(t) = \alpha^{-1}fx^*(t)z^*(t) - x^*(t)y^*(t)$ and $h(t) = y^*(t)z^*(t) + x^*(t)z^*(t) - x^*(t)y^*(t)$.

The analysis of System (12) allows us to obtain the following propositions, which give us properties on the switching function $L(\cdot)$.

Proposition 3. *The switching function L cannot vanish on any finite subinterval of $[0, T]$.*

Proof. Let us assume that there exists an interval $D \subset [0, T]$ such that for all $t \in D$, $L(t) = 0$. Then, for all $t \in D$, $\dot{L}(t) = 0$. According to the first equation of System (12), we obtain that $G(t) = 0$ for all $t \in D$. Thus, $\dot{G}(t) = 0$ for all $t \in D$. From the second equation of (12), we determine that $P(t) = 0$, for $t \in D$; thus, we have $\dot{P}(\cdot) = 0$ throughout the interval D . Consequently, the third equation of System (12) is also satisfied. We thus find

$$L(t) = 0, G(t) = 0, P(t) = 0, \forall t \in D. \quad (13)$$

Moreover, System (12) is in fact a system of non-autonomous homogeneous linear differential equations, and thus (13) holds everywhere on $[0, T]$. From (13) and the definition of $L(\cdot)$, we have $\psi_1^*(t) = 0$. Furthermore, $G(t) = 0$ implies that $\psi_1^*(t) + \psi_2^*(t) - \psi_3^*(t) = 0$; hence,

$\psi_2^*(t) = \psi_3^*(t)$. Finally, $P(t) = 0$ gives $-\psi_3^*(t) + \alpha^{-1}f\psi_2^*(t) = 0$; thus, $(1 - \alpha^{-1}f)\psi_2^*(t) = 0$. Since $f < \alpha$, we have $\alpha^{-1}f < 1$, and hence, $\psi_2^*(t) = 0$. Therefore,

$$\psi_1^*(t) = 0, \quad \psi_2^*(t) = 0, \quad \psi_3^*(t) = 0, \quad \forall t \in [0, T],$$

that is, the function $\psi^*(.)$ is trivial on $[0, T]$, which is absurd and completes the proof. $\square$

Remark 1. From (11) and Proposition 3, it follows that the control $u^*(t)$ is a piecewise constant function such that

$$u^*(t) = \begin{cases} u_{max} & \text{if } L(t) > 0, \\ 0 & \text{if } L(t) < 0. \end{cases} \quad (14)$$

Proposition 4. On the interval $[0, T]$, the switching function L has at most two zeros.

Proof. We will use the method given in [19]. The proof is carried out in three steps.

In the first step, we perform a variable change to reduce the matrix of the non-autonomous linear System (12) to an upper triangular form. The variable changes are

$$r(t) = L(t), \quad v(t) = G(t), \quad \mu(t) = P(t) + q_1(t)L(t) + q_2(t)G(t),$$

where the functions $q_1(t)$ and $q_2(t)$ will be specified later. With these variable changes, System (12) becomes

$$\begin{cases} \dot{r}(t) = u^*(t)r(t) + y^*(t)z^*(t)v(t) \\ \dot{v}(t) = (u^*(t) - \alpha q_1(t))r(t) + (h(t) - \alpha q_2(t))v(t) + \alpha \mu(t) \\ \dot{\mu}(t) = \left\{ \dot{q}_1(t) + (u(t) - \alpha)q_1(t) - \alpha q_1(t)q_2(t) + q_2(t)u(t) \right\} r(t) \\ \quad + \left\{ \dot{q}_2(t) + (h(t) - \alpha)q_2(t) - \alpha q_2^2(t) + y^*(t)z^*(t)q_1(t) \right. \\ \quad \left. + \rho(t) \right\} v(t) + \alpha(1 + q_2(t))\mu(t). \end{cases} \quad (15)$$

We choose $q_1(.)$ and $q_2(.)$ so that the expressions between braces are zero; therefore, System (15) becomes

$$\begin{cases} \dot{r}(t) = u^*(t)r(t) + y^*(t)z^*(t)v(t) \\ \dot{v}(t) = (u^*(t) - \alpha q_1(t))r(t) + (h(t) - \alpha q_2(t))v(t) + \alpha \mu(t) \\ \dot{\mu}(t) = \alpha(1 + q_2(t))\mu(t). \end{cases} \quad (16)$$

For System (16), we then make the following substitutions:

$$\hat{r}(t) = r(t), \quad \hat{v}(t) = v(t) + q_3(t)r(t) \text{ and } \hat{\mu}(t) = \mu(t),$$

where the function $q_3(.)$ will be determined later. System (16) is then rewritten as follows:

$$\begin{cases} \dot{\hat{r}}(t) = (u^*(t) - y^*(t)z^*(t)q_3(t))\hat{r}(t) + y^*(t)z^*(t)\hat{v}(t) \\ \dot{\hat{v}}(t) = \left\{ \dot{q}_3(t) + (u^*(t) - h(t))q_3(t) - y^*(t)z^*(t)q_3^2(t) \right. \\ \quad \left. + \alpha q_2(t)q_3(t) + u^*(t) - \alpha q_1(t) \right\} \hat{r}(t) + \left[h(t) - \alpha q_2(t) \right. \\ \quad \left. + y^*(t)z^*(t)q_3(t) \right] \hat{v}(t) + \alpha \hat{\mu}(t) \\ \dot{\hat{\mu}}(t) = \alpha(1 + q_2(t))\hat{\mu}(t). \end{cases} \quad (17)$$

We choose $q_3(\cdot)$ so that the expression between braces is zero; therefore, System (17) becomes

$$\begin{cases} \hat{r}(t) = [u^*(t) - y^*(t)z^*(t)q_3(t)]\hat{r}(t) + y^*(t)z^*(t)\hat{v}(t) \\ \hat{v}(t) = [h(t) - \alpha q_2(t) + y^*(t)z^*(t)q_3(t)]\hat{v}(t) + \alpha\hat{\mu}(t) \\ \hat{\mu}(t) = \alpha[1 + q_2(t)]\hat{\mu}(t). \end{cases} \quad (18)$$

By definition of $q_1(\cdot)$, $q_2(\cdot)$, and $q_3(\cdot)$, we have the following non-autonomous system of quadratic differential equations:

$$\begin{cases} \dot{q}_1(t) = (\alpha - u^*(t))q_1(t) + \alpha q_1(t)q_2(t) - u^*(t)q_2(t) \\ \dot{q}_2(t) = (\alpha - h(t))q_2(t) + \alpha q_2^2(t) - y^*(t)z^*(t)q_1(t) - \rho(t) \\ \dot{q}_3(t) = (h(t) - u^*(t))q_3(t) + y^*(t)z^*(t)q_3^2(t) - \alpha q_2(t)q_3(t) \\ \quad + \alpha q_1(t) - u^*(t). \end{cases} \quad (19)$$

The continuity of the solutions to non-autonomous systems of quadratic differential equations has been considered in [20,21], where it has been found that adding the initial conditions $q_1(0) = q_1^0$, $q_2(0) = q_2^0$, and $q_3(0) = q_3^0$ to System (19) ensures that the corresponding solution $q(\cdot) = (q_1(\cdot), q_2(\cdot), q_3(\cdot))^T$ is defined on the interval $[0, t_{\max})$, which is the largest interval on which this solution exists, with either $t_{\max} = +\infty$ or $t_{\max} < +\infty$. It is also possible that $t_{\max} \leq T$.

In the second step, we prove the existence of a solution $\tilde{q}(\cdot)$ for (19) defined over the entire interval $[0, T]$. Moreover, System (19) can be rewritten as follows:

$$\begin{cases} \dot{q}_1(t) = q^\top(t)M_1(t)q(t) + b_1^\top(t)q(t) + k_1(t), \\ \dot{q}_2(t) = q^\top(t)M_2(t)q(t) + b_2^\top(t)q(t) + k_2(t), \\ \dot{q}_3(t) = q^\top(t)M_3(t)q(t) + b_3^\top(t)q(t) + k_3(t), \end{cases} \quad (20)$$

where

$$M_1(t) = \begin{pmatrix} 0 & \frac{\alpha}{2} & 0 \\ \frac{\alpha}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_2(t) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_3(t) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\alpha}{2} \\ 0 & -\frac{\alpha}{2} & y^*(t)z^*(t) \end{pmatrix},$$

$$b_1(t) = \begin{pmatrix} \alpha - u^*(t) \\ -u^*(t) \\ 0 \end{pmatrix}, \quad b_2(t) = \begin{pmatrix} -y^*(t)z^*(t) \\ \alpha - h(t) \\ 0 \end{pmatrix}, \quad b_3(t) = \begin{pmatrix} \alpha \\ 0 \\ h(t) - u^*(t) \end{pmatrix},$$

$$k_1(t) = 0, \quad k_2(t) = -\rho(t) \quad \text{and} \quad k_3(t) = -u^*(t).$$

Now, suppose that for any arbitrary solution of System (20), $t_1 \in (0, T]$ is defined on the interval $[0, t_1)$, which is the largest interval over which this solution exists. Thus,

$$\lim_{t \rightarrow t_1^-} |q(t)| = +\infty, \quad (21)$$

where $|q(t)| = \sqrt{q_1^2(t) + q_2^2(t) + q_3^2(t)}$ here and in the following. This relation implies the existence of a real number $\rho_1 > 0$ and a $t_0 \in [0, t_1)$ such that $|q(t)| \geq \rho_1$, for all $t \in [t_0, t_1)$.

The values of ρ_1 and t_0 will be defined below.
Moreover, using the fact that

$$|q(t)|^2 = q_1^2(t) + q_2^2(t) + q_3^2(t)$$

and

$$2\left(\frac{d}{dt}|q(t)|\right)|q(t)| = 2(\dot{q}_1(t)q_1(t) + \dot{q}_2(t)q_2(t) + \dot{q}_3(t)q_3(t)),$$

we have

$$\left(\frac{d}{dt}|q(t)|\right)|q(t)| = \dot{q}_1(t)q_1(t) + \dot{q}_2(t)q_2(t) + \dot{q}_3(t)q_3(t).$$

From (20), we obtain

$$\begin{aligned} \frac{d}{dt}(|q(t)|) &= |q(t)|^{-1} \left([q_1(t)q^\top(t)M_1(t)q(t) + q_2(t)q^\top(t)M_2(t)q(t) + q_3(t)q^\top(t)M_3(t)q(t)] \right. \\ &\quad + [q_1(t)b_1^\top(t)q(t) + q_2(t)b_2^\top(t)q(t) + q_3(t)b_3^\top(t)q(t)] \\ &\quad \left. + [q_1(t)k_1(t) + q_2(t)k_2(t) + q_3(t)k_3(t)] \right) \end{aligned} \quad (22)$$

We use Proposition 1 and (2) to find an upper bound for the expressions between brackets in (22). First, we consider the expression between the third bracket of (22). Let $k(t) = (k_1(t), k_2(t), k_3(t))$. We get

$$q_1(t)k_1(t) + q_2(t)k_2(t) + q_3(t)k_3(t) = \langle k(t), q(t) \rangle \leq |k(t)||q(t)| = \sqrt{\rho(t)^2 + u^*(t)^2}|q(t)|. \quad (23)$$

But, $\rho(t)^2 = x^*(t)^2(\alpha^{-1}fz^*(t) - y^*(t))^2 \leq 2x^*(t)^2(\alpha^{-2}f^2z^*(t)^2 + y^*(t)^2)$, because $(a - b)^2 \leq 2(a^2 + b^2)$, for all $a, b \in \mathbb{R}$. Hence,

$$q_1(t)k_1(t) + q_2(t)k_2(t) + q_3(t)k_3(t) \leq C|q(t)|,$$

with $C = \sqrt{2m^2(\alpha^{-2}f^2z_{max}^2 + y_{max}^2) + u_{max}^2}$. Now, let us consider the expression between the second bracket of (22) and set $N(t) = q_1(t)b_1^\top(t)q(t) + q_2(t)b_2^\top(t)q(t) + q_3(t)b_3^\top(t)q(t)$. Then,

$$N(t) = \langle b(t), q(t) \rangle q(t) \leq |b(t)||q(t)|^2 = \sqrt{|b_1^\top(t)|^2 + |b_2^\top(t)|^2 + |b_3^\top(t)|^2}|q(t)|^2, \quad (24)$$

with $b(t) = (b_1^\top(t), b_2^\top(t), b_3^\top(t))$, that is,

$$N(t) \leq \left((\alpha - u^*(t))^2 + u^*(t)^2 + y^*(t)^2z^*(t)^2 + (\alpha - h(t))^2 + \alpha^2 + (h(t) - u^*(t))^2 \right)^{\frac{1}{2}}|q(t)|^2. \quad (25)$$

But, $y^*(t)^2z^*(t)^2 < y_{max}^2z_{max}^2$ and $(\alpha - u^*(t))^2 \leq 2\alpha^2 + 2u^*(t)^2 \leq 2\alpha^2 + 2u_{max}^2$, and hence

$$\begin{aligned} (\alpha - h(t))^2 &= \left((y^*(t)z^*(t) + x^*(t)z^*(t)) - (x^*(t)y^*(t) + d) \right)^2 \\ &\leq 4y^*(t)^2z^*(t)^2 + 4x^*(t)^2z^*(t)^2 + 4x^*(t)^2y^*(t)^2 + 4\alpha^2 \\ &\leq 4y_{max}^2z_{max}^2 + 4m^2z_{max}^2 + 4m^2y_{max}^2 + 4\alpha^2 \end{aligned} \quad (26)$$

and

$$\begin{aligned} (h(t) - u^*(t))^2 &= \left((y^*(t)z^*(t) + x^*(t)z^*(t)) - (x^*(t)y^*(t) + u^*(t)) \right)^2 \\ &\leq 4y^*(t)^2z^*(t)^2 + 4x^*(t)^2z^*(t)^2 + 4x^*(t)^2y^*(t)^2 + 4u^*(t)^2 \\ &\leq 4y_{max}^2z_{max}^2 + 4m^2z_{max}^2 + 4m^2y_{max}^2 + 4u_{max}^2. \end{aligned} \quad (27)$$

Substituting these inequalities into (25), we find

$$N(t) \leq B|q(t)|^2,$$

with $B = \sqrt{7\alpha^2 + 7u_{\max}^2 + 9y_{\max}^2 z_{\max}^2 + 8m^2 z_{\max}^2 + 8m^2 y_{\max}^2}$. Finally, we consider the expression between the first bracket of (22). Let $V(t) = q_1(t)q^\top(t)M_1(t)q(t) + q_2(t)q^\top(t)M_2(t)q(t) + q_3(t)q^\top(t)M_3(t)q(t)$. Then,

$$V(t) \leq |q_1(t)||M_1(t)q(t)||q(t)| + |q_2(t)||M_2(t)q(t)||q(t)| + |q_3(t)||M_3(t)q(t)||q(t)|.$$

We have $|M_1(t)q(t)| \leq \frac{\alpha}{2}|q(t)|$ and $|M_2(t)q(t)| \leq \alpha|q(t)|$, and the eigenvalues of the matrix $M_3(t)$ are

$$\gamma_1(t) = 0, \quad \gamma_2(t) = \frac{y^*(t)z^*(t) - \sqrt{y^*(t)^2 z^*(t)^2 + \alpha^2}}{2}$$

and

$$\gamma_3(t) = \frac{y^*(t)z^*(t) + \sqrt{y^*(t)^2 z^*(t)^2 + \alpha^2}}{2}.$$

Consequently,

$$|q^\top(t)M_3(t)q(t)| \leq \gamma_3(t)|q(t)|^2$$

and

$$\begin{aligned} V(t) &\leq \frac{\alpha}{2}|q_1(t)||q(t)|^2 + \alpha|q_2(t)||q(t)|^2 + \gamma_3(t)|q_3(t)||q(t)|^2 \\ &= \langle s(t), |q(t)| \rangle |q(t)|^2, \quad \text{with } s(t) = \left(\frac{\alpha}{2}, \alpha, \gamma_3(t) \right) \\ &\leq |s(t)||q(t)|^3 \\ &= \sqrt{\frac{\alpha^2}{4} + \alpha^2 + \frac{(y^*(t)z^*(t) + \sqrt{y^*(t)^2 z^*(t)^2 + \alpha^2})^2}{4}} |q(t)|^3, \end{aligned}$$

that is,

$$V(t) \leq A|q(t)|^3,$$

with $A = \sqrt{\frac{7\alpha^2}{4} + y_{\max}^2 z_{\max}^2}$. By substituting all the previous relations in (22), we finally obtain the following differential inequality:

$$\frac{d}{dt}(|q(t)|) \leq A|q(t)|^2 + B|q(t)| + C. \quad (28)$$

Considering the quadratic equation

$$AK^2 - BK + C = 0, \quad (29)$$

and its discriminant

$$\begin{aligned} \Delta &= (\sqrt{7\alpha^2 + 4y_{\max}^2 z_{\max}^2})^2 + (\sqrt{8m^2(\alpha^{-2}f^2 z_{\max}^2 + y_{\max}^2) + 4u_{\max}^2})^2 \\ &\quad - \sqrt{7\alpha^2 + 4y_{\max}^2 z_{\max}^2} \sqrt{8m^2(\alpha^{-2}f^2 z_{\max}^2 + y_{\max}^2) + 4u_{\max}^2} + 3u_{\max}^2 \\ &\quad + 5y_{\max}^2 z_{\max}^2 + 8m^2 z_{\max}^2 (1 - \alpha^{-2}f^2), \end{aligned}$$

and the fact that $\frac{1}{2}a^2 + \frac{1}{2}b^2 \geq ab$, for all $a, b \in \mathbb{R}$, we have

$$\Delta \geq \frac{7\alpha^2}{2} + 5u_{\max}^2 + 7y_{\max}^2 z_{\max}^2 + 4m^2 y_{\max}^2 + 4m^2 z_{\max}^2 (2 - \alpha^{-2}f^2).$$

But $f < \alpha$; thus,

$$\Delta \geq \frac{7\alpha^2}{2} + 5u_{\max}^2 + 7y_{\max}^2 z_{\max}^2 + 4m^2 y_{\max}^2 + 4m^2 z_{\max}^2 (2 - \alpha^{-2}f^2) > 0.$$

Consequently, the discriminant of Equation (29) is positive. Let K_0 be the largest root of (29):

$$K_0 = \frac{B + \sqrt{B^2 - 4AC}}{2A}.$$

For any vector $q \in \mathbb{R}^3$ such that $|q(t)| \geq \rho$, we introduce the function W such that $W(q) = |q| + K_0$. Then,

$$\begin{aligned} \frac{d}{dt}(W(q(t))) &= \frac{d}{dt}(|q(t)|) \leq A|q(t)|^2 + B|q(t)| + C \\ &= A(W(q(t)) - K_0)^2 + B(W(q(t)) - K_0) + C, \end{aligned}$$

that is, for all $t \in [t_0, t_1]$,

$$\frac{d}{dt}(W(q(t))) \leq AW(q(t))^2 - (2AK_0 - B)W(q(t)). \quad (30)$$

But, $K_0 = \frac{B + \sqrt{B^2 - 4AC}}{2A}$ implies that $2AK_0 = B + \sqrt{B^2 - 4AC}$ and $2AK_0 > B$.

Let $\phi(\cdot) = W(q(\cdot))$ and consider the auxiliary Cauchy problem

$$\begin{cases} \dot{\phi}(t) = A\phi^2(t) - (2AK_0 - B)\phi(t), & t \in [t_0, t_1] \\ \phi(t_0) = \phi_0, & \phi_0 \geq \rho + K_0. \end{cases} \quad (31)$$

We know that $A > 0$, $B > 0$, and $C > 0$, so we have $0 < B^2 - 4AC < B^2$, which implies that $\sqrt{B^2 - 4AC} < B$. This leads to $A\left(\frac{B + \sqrt{B^2 - 4AC}}{2A}\right) < B$, and thus, $AK_0 < B$. In this case, we have $2AK_0 - B < AK_0$ so $\frac{2AK_0 - B}{A} < K_0$. Thus,

$$\phi_0 \geq \rho + K_0 > K_0 > \frac{2AK_0 - B}{A}. \quad (32)$$

By solving the Bernoulli equation associated with the Cauchy problem (31), we find that for all $t \in [t_0, t_1]$,

$$\phi(t) = \left(\frac{A}{2AK_0 - B} + \left[\frac{1}{\phi_0} - \frac{A}{2AK_0 - B} \right] e^{(2AK_0 - B)(t - t_0)} \right)^{-1}. \quad (33)$$

Let us assume that ρ and t_0 are such that the expression between brackets is defined for all $t \in [t_0, t_1]$. This can be achieved, for example, by choosing t_0 for a given ρ such that the difference $(t_1 - t_0)$ is sufficiently small. From (32), the expression between brackets in (33) is negative; hence, $\phi(\cdot)$ is a finite positive function that increases on $[t_0, t_1]$. Therefore, we have $\phi(t) < \phi(t_1)$ for all $t \in [t_0, t_1]$. Consequently, from the differential inequality (30), the Cauchy problem (31), Theorem 6.1 of Chapter 1 in [22], and

$$\phi_0 = W(q(t_0)) = |q(t_0)| + K_0,$$

we get $W(q(t)) \leq \phi(t)$, which implies that $|q(t)| + K_0 \leq \phi(t)$, and thus, $|q(t)| \leq \phi(t) - K_0 < \phi(t_1) - K_0$, $t \in (t_0, t_1)$, which is in contradiction with (21). Therefore, there exists a solution $\tilde{q}(t)$ of (19) which is defined on the entire interval $[0, T]$. Thus, (18) is also defined on this interval.

Rewriting the system using the components of $\tilde{q}(t)$,

$$\begin{cases} \dot{\hat{r}}(t) = (u^*(t) - y^*(t)z^*(t)\tilde{q}_3(t))\hat{r}(t) + y^*(t)z^*(t)\hat{v}(t) \\ \dot{\hat{v}}(t) = (h(t) - \alpha\tilde{q}_2(t) + y^*(t)z^*(t)\tilde{q}_3(t))\hat{v}(t) + \alpha\hat{\mu}(t) \\ \dot{\hat{\mu}}(t) = \alpha(1 + \tilde{q}_2(t))\hat{\mu}(t), \end{cases} \quad (34)$$

in a third step and with (34), we show that the function $\hat{r}(t) = L(t)$ has at most two distinct zeros. Let us assume that $\hat{r}(t)$ has at least three distinct zeros τ_1, τ_2, τ_3 on $[0, T]$ such that $0 < \tau_1 < \tau_2 < \tau_3 < T$. Applying the generalized Rolle's theorem [23] to the first equation of (34), we conclude that the function $\hat{v}(t)$ has at least two distinct zeros σ_1, σ_2 on $(0, T)$ such that $0 < \sigma_1 < \sigma_2 < T$. Similarly, applying the generalized Rolle's theorem to the second equation of (34), we obtain that the function $\hat{\mu}(t)$ has at least one zero ξ on $(0, T)$. But, according to the third equation of (34), $\hat{\mu}(t) = \hat{\mu}_0 \exp\left(\alpha \int_0^t (\alpha + \tilde{q}_2(s))ds\right)$, and hence, $\hat{\mu}(t) = 0$ everywhere on $[0, T]$. Returning to the second equation of (34), we find that $\hat{v}(t) = 0$ everywhere on $[0, T]$ and the first equation of (34) leads to the same conclusion for the function $\hat{r}(t)$, that is, $\hat{r}(t) = 0$, for all $t \in [0, T]$. This is in contradiction with Lemma 3. Consequently, the switching function $L(\cdot)$ has at most two distinct zeros on $[0, T]$. $\square$

Proposition 5. *There exists $\theta \in [0, T)$ such that the optimal control $u^*(\cdot)$ satisfies $u^*(t) = u_{max}$ for all $t \in (\theta, T)$.*

Proof. This proposition is a consequence of the two previous ones. $\square$

Remark 2. *From Propositions 4 and 5 and the initial conditions of System (12) and (14), we characterize the optimal control $u^*(\cdot)$. It can either be a constant function $u^*(t) = u_{max}$, for all $t \in [0, T]$, or a piecewise constant function such that*

$$u^*(t) = \begin{cases} 0 & \text{if } 0 \leq t \leq \theta^*, \\ u_{max} & \text{if } \theta^* < t \leq T, \end{cases} \quad (35)$$

where $\theta^* \in [0, T)$ is the switching time.

2.2. Study of the Optimal Control Problem ($\tilde{\mathcal{P}}$)

By applying the Pontryagin maximum principle, we will characterize the optimal control $\tilde{u}^*$ associated with the optimal control problem ($\tilde{\mathcal{P}}$). For the control $\tilde{u}^*(t)$ and the corresponding solution $\tilde{X}^*(t) = (\tilde{x}^*(t), \tilde{y}^*(t), \tilde{z}^*(t))^\top$, there exists a non-trivial solution $\tilde{\psi}^*(t) = (\tilde{\psi}_1^*(t), \tilde{\psi}_2^*(t), \tilde{\psi}_3^*(t))$ of the adjoint system

$$\begin{cases} \dot{\tilde{\psi}}_1^*(t) = \tilde{u}^*(t)\tilde{\psi}_1^*(t) + \tilde{y}^*(t)\tilde{z}^*(t)(\tilde{\psi}_1^*(t) + \tilde{\psi}_2^*(t) - \tilde{\psi}_3^*(t)) \\ \dot{\tilde{\psi}}_2^*(t) = \tilde{x}^*(t)\tilde{z}^*(t)(\tilde{\psi}_1^*(t) + \tilde{\psi}_2^*(t) - \tilde{\psi}_3^*(t)) + 1 \\ \dot{\tilde{\psi}}_3^*(t) = \tilde{x}^*(t)\tilde{y}^*(t)(\tilde{\psi}_1^*(t) + \tilde{\psi}_2^*(t) - \tilde{\psi}_3^*(t)) + \alpha\tilde{\psi}_3^*(t) - f\tilde{\psi}_2^*(t) \\ \tilde{\psi}_1^*(T) = 0, \tilde{\psi}_2^*(T) = 0, \tilde{\psi}_3^*(T) = 0, \end{cases} \quad (36)$$

such that the control $\tilde{u}^*(t)$ maximizes the Hamiltonian $\tilde{\mathcal{H}}$ defined by

$$\tilde{\mathcal{H}}(x, y, z, \psi_1, \psi_2, \psi_3, \tilde{u}) = -y + (-xyz + \tilde{u}(m - x))\psi_1 + (-xyz + fz)\psi_2 + (xyz - \alpha z)\psi_3.$$

But, $0 \leq \tilde{u}^*(t) \leq \tilde{u}_{max}$, for almost all $t \in [0, T]$, so

$$\tilde{u}^*(t) = \begin{cases} \tilde{u}_{max} & \text{if } \tilde{L}(t) > 0 \\ \tilde{u}^* \in [0, \tilde{u}_{max}] & \text{if } \tilde{L}(t) = 0 \\ 0 & \text{if } \tilde{L}(t) < 0, \end{cases} \quad (37)$$

where $\tilde{L}(t) = \tilde{\psi}_1^*(t)$ is the switching function of problem $(\tilde{P})$.

In order to study the behaviour of the switching function $\tilde{L}(\cdot)$, we introduce the following auxiliary functions:

$$\tilde{G}(t) = \tilde{\psi}_1^*(t) + \tilde{\psi}_2^*(t) - \tilde{\psi}_3^*(t) \text{ and } \tilde{P}(t) = -\tilde{\psi}_3^*(t) + \alpha^{-1}f\tilde{\psi}_2^*(t) + \alpha^{-1}.$$

Now, the adjoint System (36) for problem $(\tilde{P})$ can be rewritten as the following system of equations:

$$\begin{cases} \dot{\tilde{L}}(t) = \tilde{u}^*(t)\tilde{L}(t) + \tilde{y}^*(t)\tilde{z}^*(t)\tilde{G}(t) \\ \dot{\tilde{G}}(t) = \tilde{u}^*(t)\tilde{L}(t) + \tilde{h}(t)\tilde{G}(t) + \alpha\tilde{P}(t) \\ \dot{\tilde{P}}(t) = \tilde{\rho}(t)\tilde{G}(t) + \alpha\tilde{P}(t) + \alpha^{-1}f - 1 \\ \tilde{L}(T) = 0, \tilde{G}(T) = 0, \tilde{P}(T) = \alpha^{-1}, \end{cases} \quad (38)$$

where $\tilde{\rho}(t) = \alpha^{-1}f\tilde{x}^*(t)\tilde{z}^*(t) - \tilde{x}^*(t)\tilde{y}^*(t)$ and $\tilde{h}(t) = \tilde{y}^*(t)\tilde{z}^*(t) + \tilde{x}^*(t)\tilde{z}^*(t) - \tilde{x}^*(t)\tilde{y}^*(t)$. The analysis of the Cauchy problem (38) allows us to obtain the following propositions which give properties on the switching function $\tilde{L}(\cdot)$.

Proposition 6. *The switching function $\tilde{L}(\cdot)$ is not zero on any finite subinterval of $[0, T]$.*

Proof. This proof is exactly the same than the one for Proposition 3 using System (38) and the fact that $f \neq \alpha$. $\square$

Remark 3. *From (37) and Proposition 6, it follows that the control $\tilde{u}^*(\cdot)$ is a piecewise constant function:*

$$\tilde{u}^*(t) = \begin{cases} \tilde{u}_{max} & \text{if } \tilde{L}(t) > 0, \\ 0 & \text{if } \tilde{L}(t) < 0. \end{cases} \quad (39)$$

Proposition 7. *The switching function $\tilde{L}(\cdot)$ only takes positive values on $[0, T]$.*

Proof. The proof for this lemma is carried out in several steps similarly to that for Proposition 4. In the first step, we perform a variable change to reduce the matrix of the non-autonomous linear System (38) to an upper triangular form:

$$r_1(t) = \tilde{L}(t), \quad v_1(t) = \tilde{G}(t), \quad \mu_1(t) = \tilde{P}(t) + g_1(t)\tilde{L}(t) + g_2(t)\tilde{G}(t),$$

where the functions $g_1(t)$ and $g_2(t)$ will be defined later. Using (38), we have

$$\begin{cases} \dot{r}_1(t) = \tilde{u}^*(t)r_1(t) + \tilde{y}^*(t)\tilde{z}^*(t)v_1(t) \\ \dot{v}_1(t) = (\tilde{u}^*(t) - \alpha g_1(t))r_1(t) + (\tilde{h}(t) - \alpha g_2(t))v_1(t) + \alpha\mu_1(t) \\ \dot{\mu}_1(t) = \left\{ \begin{aligned} &g_1(t) + (\tilde{u}^*(t) - \alpha)g_1(t) - \alpha g_1(t)g_2(t) + g_2(t)\tilde{u}^*(t) \\ &+ \left\{ g_2(t) + (\tilde{h}(t) - \alpha)g_2(t) - \alpha g_2^2(t) + \tilde{y}^*(t)\tilde{z}^*(t)g_1(t) \right. \\ &\left. + \tilde{\rho}(t) \right\} v_1(t) + \alpha(1 + g_2(t))\mu_1(t) + \alpha^{-1}f - 1. \end{aligned} \right\} r_1(t) \end{cases} \quad (40)$$

Choosing $g_1(\cdot)$ and $g_2(\cdot)$ such that the expressions between braces are zero, System (40) becomes

$$\begin{cases} \dot{r}_1(t) = \tilde{u}^*(t)r_1(t) + \tilde{y}^*(t)\tilde{z}^*(t)v_1(t) \\ \dot{v}_1(t) = (\tilde{u}^*(t) - \alpha g_1(t))r_1(t) + (\tilde{h}(t) - \alpha g_2(t))v_1(t) + \alpha\mu_1(t) \\ \dot{\mu}_1(t) = \alpha(1 + g_2(t))\mu_1(t) + \alpha^{-1}f - 1. \end{cases} \quad (41)$$

Then, we make the following substitutions:

$$\hat{r}_1(t) = r_1(t), \quad \hat{v}_1(t) = v_1(t) + g_3(t)r_1(t), \quad \hat{\mu}_1(t) = \mu_1(t),$$

where the function $g_3(\cdot)$ will be determined later. System (41) is rewritten as follows:

$$\begin{cases} \dot{\hat{r}}_1(t) = (\tilde{u}^*(t) - \tilde{y}^*(t)\tilde{z}^*(t)g_3(t))\hat{r}_1(t) + \tilde{y}^*(t)\tilde{z}^*(t)\hat{v}_1(t) \\ \dot{\hat{v}}_1(t) = \left\{ \begin{aligned} &g_3(t) + (\tilde{u}^*(t) - \tilde{h}(t))g_3(t) - \tilde{y}^*(t)\tilde{z}^*(t)g_3^2(t) \\ &+ \alpha g_2(t)g_3(t) + \tilde{u}^*(t) - \alpha g_1(t) \end{aligned} \right\} \hat{r}_1(t) + [\tilde{h}(t) - \alpha g_2(t) \\ + \tilde{y}^*(t)\tilde{z}^*(t)g_3(t)]\hat{v}_1(t) + \alpha\hat{\mu}_1(t) \\ \dot{\hat{\mu}}_1(t) = \alpha(1 + g_2(t))\hat{\mu}_1(t) + \alpha^{-1}f - 1. \end{cases} \quad (42)$$

We choose the function $g_3(\cdot)$ such that the expression between braces is zero; thus, System (42) becomes

$$\begin{cases} \dot{\hat{r}}_1(t) = (\tilde{u}^*(t) - \tilde{y}^*(t)\tilde{z}^*(t)g_3(t))\hat{r}_1(t) + \tilde{y}^*(t)\tilde{z}^*(t)\hat{v}_1(t) \\ \dot{\hat{v}}_1(t) = (\tilde{h}(t) - \alpha g_2(t) + \tilde{y}^*(t)\tilde{z}^*(t)g_3(t))\hat{v}_1(t) + \alpha\hat{\mu}_1(t) \\ \dot{\hat{\mu}}_1(t) = \alpha(1 + g_2(t))\hat{\mu}_1(t) + \alpha^{-1}f - 1. \end{cases} \quad (43)$$

By definition of $g_1(\cdot)$, $g_2(\cdot)$, and $g_3(\cdot)$, we have the following non-autonomous system of quadratic differential equations:

$$\begin{cases} \dot{g}_1(t) = (\alpha - \tilde{u}^*(t))g_1(t) + \alpha g_1(t)g_2(t) - \tilde{u}^*(t)g_2(t) \\ \dot{g}_2(t) = (\alpha - \tilde{h}(t))g_2(t) + \alpha g_2^2(t) - \tilde{y}^*(t)\tilde{z}^*(t)g_1(t) - \tilde{\rho}(t) \\ \dot{g}_3(t) = (\tilde{h}(t) - \tilde{u}^*(t))g_3(t) + \tilde{y}^*(t)\tilde{z}^*(t)g_3^2(t) - \alpha g_2(t)g_3(t) \\ + \alpha g_1(t) - \tilde{u}^*(t). \end{cases} \quad (44)$$

As in the proof of Proposition 4, by adding the initial conditions $g_1(0) = g_1^0, g_2(0) = g_2^0, g_3(0) = g_3^0$ to System (44), the corresponding solution $g(\cdot) = (g_1(\cdot), g_2(\cdot), g_3(\cdot))^T$ is defined on the interval $[0, t_{max})$, which is the largest interval on which this solution exists, with either $t_{max} = +\infty$ or $t_{max} < +\infty$. In the second step, we prove the existence of a solution $g(\cdot)$ to System (44) defined on the entire interval $[0, T]$.

The proof is similar to that for the existence of a solution to System (19) of Problem (P) in Proposition 4.

Solving the third equation of (43), we find that

$$\begin{aligned}\hat{\mu}_1(t) &= \exp\left(\alpha \int_T^t (1 + g_2(\epsilon)) d\epsilon\right) \times \\ &\quad \left(\hat{\mu}_1(T) + (\alpha^{-1}f - 1) \int_T^t \exp\left(-\alpha \int_T^s (1 + g_2(\epsilon)) d\epsilon\right) ds\right).\end{aligned}\quad (45)$$

Since $\hat{\mu}_1(T) = \mu_1(T) = \tilde{P}(T) + g_1(T)\tilde{L}(T) + \tilde{G}(T) = \alpha^{-1}$, then

$$\hat{\mu}_1(t) = e^{-\alpha \int_t^T (1 - g_2(\epsilon)) d\epsilon} \left(\alpha^{-1} + (1 - \alpha^{-1}f) \int_t^T e^{-\alpha \int_t^s (1 - g_2(\epsilon)) d\epsilon} ds\right).$$

Hence, $\hat{\mu}_1(t) > 0$, for all $t \in [0, T]$. Now, the second equation of (43) gives

$$\begin{aligned}\hat{v}_1(t) &= \exp\left(\int_T^t (\tilde{h}(\epsilon) - \alpha \tilde{g}_2(\epsilon) + \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \times \\ &\quad \left(\hat{v}_1(T) + \alpha \int_T^t \exp\left(-\int_T^s (\tilde{h}(\epsilon) - \alpha \tilde{g}_2(\epsilon) + \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \hat{\mu}_1(s) ds\right).\end{aligned}$$

Since $\hat{v}_1(T) = \tilde{G}(T) + g_3(T)\tilde{L}(T) = 0$ then

$$\hat{v}_1(t) = -\alpha \int_t^T \exp\left(-\int_t^s (\tilde{h}(\epsilon) - \alpha \tilde{g}_2(\epsilon) + \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \hat{\mu}_1(s) ds.$$

Hence, $\hat{v}_1(t) < 0$, for all $t \in [0, T]$. Finally, with the first equation of (43), we get

$$\begin{aligned}\hat{r}_1(t) &= \exp\left(\int_T^t (\tilde{u}^*(\epsilon) - \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \times \\ &\quad \left(\hat{r}_1(T) + \int_T^t \exp\left(-\int_T^s (\tilde{u}^*(\epsilon) - \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \tilde{y}^*(s)\tilde{z}^*(s)\hat{v}_1(s) ds\right).\end{aligned}$$

Since $\hat{r}_1(T) = r_1(T) = \tilde{L}(T) = 0$,

$$\hat{r}_1(t) = -\int_t^T \exp\left(-\int_t^s (\tilde{u}^*(\epsilon) - \tilde{y}^*(\epsilon)\tilde{z}^*(\epsilon)\tilde{g}_3(\epsilon)) d\epsilon\right) \tilde{y}^*(s)\tilde{z}^*(s)\hat{v}_1(s) ds.$$

Hence, $\hat{r}_1(t) > 0$, for all $t \in [0, T]$, which implies that $\tilde{L}(t) > 0$, for all $t \in [0, T]$. $\square$

Remark 4. According to Proposition 7 and (39), the optimal control $\tilde{u}^*(t)$ satisfies

$$\tilde{u}^*(t) = \tilde{u}_{max}, \quad \forall t \in [0, T]. \quad (46)$$

2.3. Numerical Simulations

We used MATLAB R2015a (8.5.0.197613) on a computer with an AMD RYZEN 7 processor at 3.9 GHz and 8 GB of RAM to make simulations.

For problem (P), we considered $\alpha = 0.5000$, $f = 0.0100$, $m = 2$, and $T = 50$, and the initial conditions were $x_0 = 10$, $y_0 = 30$, and $z_0 = 0.9999$. These numerical values were obtained from [13], to which we simply added a value for f satisfying $f < \alpha$. A global minimum has been obtained on $[0, T]$ with $\theta^* = 10$ as well as the minimum value of the cost function $y(50) = 0.0050016$ (see Figure 1), which is compatible with our previous

theoretical results (see Remark 2). Moreover, with the obtained optimal control, we can see that the concentration of pollutants significantly decreases.

Figure 1 illustrates the evolution of pollutants, bacteria, and oxygen concentrations with the optimal control $u^*(\cdot)$ defined in (35). At the beginning of the reaction in the interval $[0, 10]$, it can be seen that the oxygen concentration decreases due to its consumption by the bacteria. Indeed, due to the lack of oxygen and their low initial concentration, the bacteria fail to consume all the pollutants initially introduced in the reactor, resulting in their decrease. During this time interval, only about 33% of the initially introduced pollutants are consumed by the bacteria. From $t = 10$ onwards, the oxygen concentration increases due to air pumping, and at this point, the bacteria concentration begins to increase quickly, while the pollutant concentration decreases significantly, and for sufficiently large t values, the pollutant concentration tends to zero.

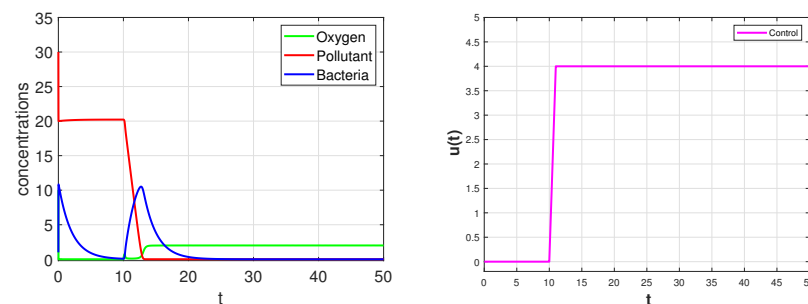


Figure 1. Evolution of pollutants, bacteria, and oxygen concentrations (left) and the optimal control (right).

For problem $(\tilde{P})$, following Propositions 6 and 7, we are able to determine the type of optimal control. According to Remark 4, we have $\tilde{u}^*(t) = \tilde{u}_{max}$ for all $t \in [0, T]$. Here, we consider $\alpha = 1$, $f = 0.24$, $m = 2$, and $u_{max} = 4$, and the initial conditions are $x_0 = 12$, $y_0 = 14$, $z_0 = 0.9999$, and $T = 2$.

Figure 2 illustrates the evolution of the concentrations of oxygen, pollutants, and bacteria in the reactor, as well as the outcome of minimizing the cost function $\int_0^2 y(t)dt$. It can be seen that at the beginning of the reaction, the oxygen concentration (in green) decreases quickly, which is due to its use by bacteria. Additionally, there is a point at which the oxygen concentration starts to increase, which is due to the decreased consumption by bacteria as they die from a lack of substrates. We can also remark that the concentration of pollutants (in red) decreases significantly, and for sufficiently large values of t , its trajectory tends towards zero. Furthermore, the concentration of bacteria (in blue) initially increases quickly but starts to decrease due to the reduction in the substrates (pollutants) needed for their metabolism.

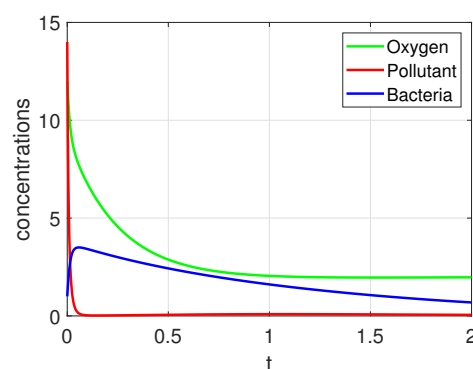


Figure 2. Evolution of the controlled system.

3. Study of an Optimal Control Problem for a Wastewater Treatment Model with Two Types of Bacteria

In this section, we modify model (1) by considering two types of bacteria, mesophilic and thermophilic bacteria, as is the case in wastewater treatment [14]. We consider an optimal control problem in order to minimize the weighted sum of pollutant concentration at the final time and the costs of oxygen pumping operation.

3.1. Mathematical Model of the Aerobic Digestion Process

A mathematical model of this process can be formulated as a system of four ordinary differential equations:

$$\begin{cases} \dot{x}(t) = -x(t)y(t)z(t) - ax(t)y(t)w(t) - bx(t)z(t)w(t) + U(t)(m - x(t)), \\ \dot{y}(t) = -x(t)y(t)z(t) - cx(t)y(t)w(t) + rz(t) + kw(t) - \lambda y(t), \\ \dot{z}(t) = x(t)y(t)z(t) - \alpha x(t)z(t)w(t) - \sigma z(t), \\ \dot{w}(t) = x(t)y(t)w(t) + ex(t)z(t)w(t) - fw(t), \\ x(0) = x_0 \in (0, m), y(0) = y_0 > 0, z(0) = z_0 > 0, w(0) = w_0 > 0. \end{cases} \quad (47)$$

Here, $x(\cdot)$ is the concentration of oxygen, $y(\cdot)$ the concentration of organic matter (pollutants), $z(\cdot)$ the concentration of mesophilic aerobic bacteria, and $w(\cdot)$ the concentration of thermophilic aerobic bacteria. This model assumes that the reaction is described by the law of mass action.

System (47) is considered over a fixed time interval $[0, T]$, which corresponds to the duration of a single batch treatment.

The first equation of the system describes the evolution of oxygen concentration in the treated sludge: the first, second, and third terms describe its consumption in the reaction and the fourth term describes the input of oxygen (through pumping) into the reactor from the outside. Dissolved oxygen is replenished by pumping, which is subject to the saturation concentration m . Here, $U(\cdot)$ represents the oxygen pumping rate, which also serves as the control function for this model. The second equation describes the evolution of pollutant concentration, the first two terms describe their degradation by the two bacteria types and the third and fourth terms describe the production of pollutants due to the decomposition of mesophilic and thermophilic bacteria, of which a fraction of r and k is, respectively, recycled as substrates. Pollutants naturally degrade at a rate λ . The third equation describes the evolution of mesophilic aerobic bacteria; the first term defines their growth, the second term defines their reduction due to the growth of thermophilic bacteria, and the mesophilic bacteria also die naturally at a rate σ . Finally, the fourth equation describes the growth of thermophilic aerobic bacteria; the first term defines their growth by consuming organic pollutants, the second term defines their growth due to the reduction in mesophilic bacteria, and they also die naturally at a rate f . Moreover, a, b, c, α, e are positive rate constants of the mass action law and k, r, σ, f are positive real numbers. Consequently, according to the definition of all these parameters, it is natural to consider that

$$k < f, \quad r < \sigma, \quad f < \sigma. \quad (48)$$

System (47) is a controlled system with the function $U(\cdot)$ as control. The set of corresponding admissible controls is composed of all Lebesgue measurable functions $U(\cdot)$ such that, for almost every $t \in [0, T]$,

$$0 \leq U(t) \leq U_{\max}, \quad (49)$$

where $U_{\max}$ is the maximum aeration rate. For any $U \in [0, U_{\max}]$, we set $u = \frac{U}{U_{\max}}$. The set of admissible controls for u is

$$\mathcal{U} := \left\{ v : [0, T] \longrightarrow [0, 1], v \text{ Lebesgue measurable} \right\} \quad (50)$$

and System (47) becomes

$$\begin{cases} \dot{x}(t) = -x(t)y(t)z(t) - ax(t)y(t)w(t) - bx(t)z(t)w(t) + u(t)(m - x(t)), \\ \dot{y}(t) = -x(t)y(t)z(t) - cx(t)y(t)w(t) + rz(t) + kw(t) - \lambda y(t), \\ \dot{z}(t) = x(t)y(t)z(t) - \alpha x(t)z(t)w(t) - \sigma z(t), \\ \dot{w}(t) = x(t)y(t)w(t) + ex(t)z(t)w(t) - fw(t), \\ x(0) = x_0 \in (0, m), y(0) = y_0 > 0, z(0) = z_0 > 0, w(0) = w_0 > 0. \end{cases} \quad (51)$$

We want to minimize the following objective function:

$$\mathcal{J}(u) = \beta \int_0^T u^2(t) dt + y(T), \quad \beta > 0 \quad (52)$$

subject to the constraint of the dynamic associated with (51).

Proposition 8. For all control $u(\cdot) \in \mathcal{U}$, all trajectories $x(\cdot)$, $y(\cdot)$, $z(\cdot)$, and $w(\cdot)$ of (51) starting in the positive orthant are bounded and satisfy, for all $t \geq 0$,

$$0 < x(t) < m, \quad 0 < y(t) < y_{\max}, \quad 0 < w(t) < w_{\max}, \quad 0 < z(t) < z_{\max}, \quad (53)$$

where

$$y_{\max} = y_0 + z_0 + kw_{\max}T, \quad z_{\max} = x_0 + z_0 + mT, \quad w_{\max} = a^{-1}(x_0 + aw_0 + mT) \exp(emz_{\max}T).$$

Proof. The proof for this proposition is similar to that for Proposition 1. $\square$

Proposition 9. Problems (51) and (52) are well posed in the sense that for each control $u \in \mathcal{U}$, there is a unique $X = (x, y, z, w)^\top$ solution to the Cauchy problem (51).

Proof. The proof for this proposition is similar to that for Proposition 2. $\square$

Theorem 2. Problems (51) and (52) admit an optimal control $u^* \in \mathcal{U}$ such that the associated trajectory $X^* = (x^*, y^*, z^*, w^*)^\top$ is a solution of (51).

Proof. It is a consequence of the two previous propositions and the fact that the right-hand side of the equations of the model and the term under the integral of the objective function are convex with respect to u . $\square$

3.2. Pontryagin Maximum Principle

The aim of this section is to identify the necessary conditions of optimality for an optimal pair $(u^*, (x^*, y^*, z^*, w^*)^\top)$ of problems (51) and (52). For this purpose, we apply the Pontryagin maximum principle [18].

Theorem 3. Let u^* be the optimal control and $(x^*, y^*, z^*, w^*)^\top$ the trajectory associated with problems (51) and (52). There is an absolutely continuous non-trivial solution $\psi = (\psi_1, \psi_2, \psi_3, \psi_4) : [0, T] \rightarrow \mathbb{R}^4$ satisfying, for almost all $t \in [0, T]$,

$$\begin{cases} \dot{\psi}_1(t) = u^*(t)\psi_1(t) + y^*(t)z^*(t)(\psi_1(t) + \psi_2(t) - \psi_3(t)) \\ \quad + y^*(t)w^*(t)(a\psi_1(t) + c\psi_2(t) - \psi_4(t)) \\ \quad + z^*(t)w^*(t)(b\psi_1(t) + \alpha\psi_3(t) - e\psi_4(t)) \\ \dot{\psi}_2(t) = x^*(t)z^*(t)(\psi_1(t) + \psi_2(t) - \psi_3(t)) \\ \quad + x^*(t)w^*(t)(a\psi_1(t) + c\psi_2(t) - \psi_4(t)) - \lambda\psi_2(t) \\ \dot{\psi}_3(t) = x^*(t)y^*(t)(\psi_1(t) + \psi_2(t) - \psi_3(t)) + x^*(t)w^*(t)(b\psi_1(t) \\ \quad + \alpha\psi_3(t) - e\psi_4(t)) + \sigma\psi_3(t) - r\psi_2(t) \\ \dot{\psi}_4(t) = x^*(t)y^*(t)(a\psi_1(t) + c\psi_2(t) - \psi_4(t)) + x^*(t)z^*(t)(b\psi_1(t) \\ \quad + \alpha\psi_3(t) - e\psi_4(t)) + f\psi_4(t) - k\psi_2(t), \end{cases} \quad (54)$$

such that the control $u^*(t)$ maximizes the Hamiltonian $\mathcal{H}$ defined by

$$\begin{aligned} \mathcal{H}(t, X, \psi, u) = & -\beta u^2 + (u(m - x) - xyz - axyw - bxzw)\psi_1 \\ & + (rz + kw - xyz - cxyw - \lambda y)\psi_2 \\ & + (xyz - \alpha xzw - \sigma z)\psi_3 + (xyw + exzw - fw)\psi_4. \end{aligned}$$

Moreover, the transversality condition is given by

$$\psi(T) = (\psi_1(T), \psi_2(T), \psi_3(T), \psi_4(T)) = (0, -1, 0, 0).$$

Noting that the Hamiltonian is concave with respect to u , a global maximum then exists and is achieved for u^* such that

$$\frac{\partial \mathcal{H}}{\partial u}(t, X^*(t), \psi(t), u^*(t)) = 0.$$

In this case, we get

$$u^*(t) = \frac{(m - x^*(t))\psi_1(t)}{2\beta}. \quad (55)$$

Since $u^* \in \mathcal{U}$, we conclude that, for all $t \in [0, T]$,

$$u^*(t) = \min \left(1, \max \left(0, \frac{(m - x^*(t))\psi_1(t)}{2\beta} \right) \right). \quad (56)$$

3.3. Numerical Simulations

For the simulations, we chose the following values for the parameters of (51):

$$e = 0.2100, \quad c = 0.1800, \quad a = 0.0130, \quad b = 0.0150, \quad \alpha = 0.1400, \quad \sigma = 0.2400,$$

$$m = 2, \quad \lambda = 0.2000, \quad r = 0.00240, \quad \gamma = 0.0019, \quad f = 0.1900$$

We considered the weighting factor associated with the oxygen pumping cost as $\beta = 0.21$ and the initial values are $x_0 = 10$, $y_0 = 14$, $z_0 = 4$, and $w_0 = 2$.

Figure 3 illustrates the evolution of the concentrations of the different components of the system. Initially, we observe that the oxygen concentration (in green) decreases rapidly and reaches zero, then increases until the final time. The pollutant concentration (in red) decreases until the final time, and for a sufficiently large value of T , this concentration

tends towards zero. The density of mesophilic bacteria (in blue) starts to increase and then decreases, reaching zero for a sufficiently large value of T . Additionally, we notice that the concentration of thermophilic bacteria (in pink) initially increases and then decreases until the final time, so that for large time values, the thermophilic bacteria concentration is minimal.

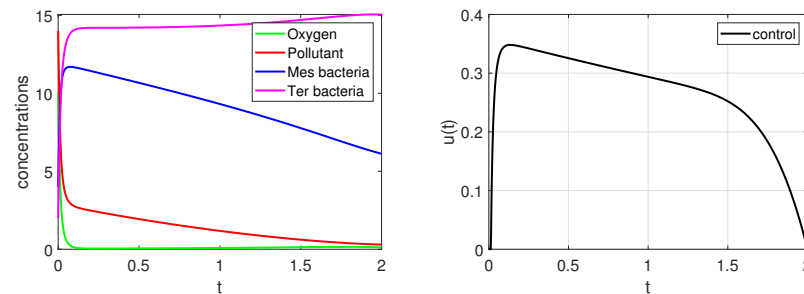


Figure 3. Evolution of concentrations (left) and the optimal control (right).

The second scheme of Figure 3 illustrates the control $u^*(.)$. It starts at its minimum value of zero, increases to 0.35, and then begins to decrease slowly.

4. Concluding Remarks

In this work, we proposed two models for wastewater treatment using aerobic bacteria, in which mesophilic and thermophilic bacteria are used to degrade organic pollutants in the presence of oxygen. First, we proposed a wastewater treatment model using only thermophilic aerobic bacteria, and for this model, we studied two different optimal control problems where the control is the oxygen injection rate in the reactor. In the second part of this paper, we proposed another wastewater treatment model using two types of aerobic bacteria, mesophilic and thermophilic ones. We proposed an optimal control problem where the control remains the oxygen injection rate. The aim of this problem is to minimize the concentration of pollutants and reduce the costs associated with oxygen pumping. An optimal control has been found for each problem and our results have been illustrated with numerical simulations.

A direct continuation of this work is the consideration of a mathematical model with a finite number (more than two) of bacteria and its optimal control study to reduce the quantity of pollutants after wastewater treatment. Moreover, in this work, we made certain numerical value choices, leading us to highlight our theoretical study, but other choices are also possible. In particular, we are waiting for real data from fellow chemists to point out the efficiency of our study. Another perspective of this work involves the reduction in oxygenation costs by introducing algae in the water to provide the necessary oxygen to bacteria to remove pollutants.

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