Modeling and optimization of activated sludge bioreactors for wastewater treatment taking into account spatial inhomogeneities

Maria Crespo, Benjamin Ivorra, Angel Manuel Ramos, Alain Rapaport

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M. Crespo[a,b,c,*], B. Ivorra[a], A.M. Ramos[a], A. Rapaport[b]

[a] *Departamento de Matemática Aplicada & Instituto de Matemática Interisciplinar, Universidad Complutense de Madrid. Plaza de Ciencias, 3, 28040 Madrid, Spain.*
[b] *UMR MISTEA - Mathématiques,Informatique et Statistique pour l´Environnement et l´Agronomie (INRA/SupAgro). 2, Place P.Viala, 34060 Montpellier, France.*
[c] *Université Montpellier, Labex Numev. 161, rue Ada, 34095 Montpellier Cedex 5, France.*

Abstract

In this work, we study optimal and suboptimal control strategies for the treatment of a polluted water resource by using aside a continuous bioreactor. The control consists in choosing the inlet volumetric flow rate for filling the bioreactor with contaminated water from a considered resource (lake, reservoir, watertable...). The treated outflow returns to the resource. We tackle an optimization problem which aims to minimize the time needed to reach a prescribed minimal value of contamination in the resource by choosing the input flow. Next, we study the influence of inhomogeneities of concentrations in the bioreactor, considering a system based on partial differential equations which describe its dynamics. We show that applying the optimal feedback control derived for perfectly mixed bioreactor does not allow to reach the target with small diffusion parameters as it drives the bioreactor to washout (the bioreactor equilibrium with no biomass). In this case, a suboptimal feedback (which reaches the target in finite time) is obtained with the help of a Hybrid Genetic Algorithm. Furthermore, we consider that the fluid flow velocity of the water entering into the bioreactor follows either a uniform or a nonuniform profile, showing that the optimal volumetric flow rates obtained with the uniform profile are not optimal if the profile is nonuniform, even when high diffusion coefficients are considered in the model.

Keywords: water treatment, bioreactor, advection diffusion reaction model, optimal control

*Corresponding author
Email addresses: mcresp01@ucm.es (M. Crespo), ivorra@mat.ucm.es (B. Ivorra), angel@mat.ucm.es (A.M. Ramos), alain.rapaport@inra.fr (A. Rapaport)

1. Introduction

The decontamination of water resources is a major environmental issue in the areas of prevention of eutrophication and wastewater treatment. Eutrophication is a process whereby water resources becomes too rich in organic material and mineral nutrients. Household products (phosphorus detergents) and products used in agriculture (nitrate fertilizers) are the main causes of pollution of water resources. As a result, some plants (in particular planktonic algae) can grow rapidly and reduce the available oxygen of the aquatic ecosystem resulting, for instance, in the death of local bio-organisms (such as fishes). The *activated sludge process* is a way of eliminating eutrophication from water resources. The process uses biomass (i.e., bacteria) to feed with substrate (i.e., the organic contaminant) in wastewater, producing a high quality effluent for a reasonable operating and maintenance cost. It consists of several interrelated components:

- A tank where the biological reaction occurs, called bioreactor. Bacteria thrive as they travel through the bioreactor and they multiply rapidly with sufficient food (substrate).
- A waste water source that feeds the bioreactor.
- A settler situated at the bottom of the bioreactor, separating bacteria from the clearer water. This accumulated bacteria is called *activated sludge*.
- A means of collecting the activated sludge, either to return it to the bioreactor or to remove it from the process.

The optimization of activated sludge processes has received a great attention in the literature (see, e.g.,[1], [2] and [3] for reviews of the different optimization techniques that have been used in bioprocesses). The objective is usually to control the inlet flow rate of the bioreactor for attaining a prescribed target (e.g., a small prescribed amount of pollutant at the bioreactor outlet) in a finite given time. Particularly, the maximization of bacteria production in a well mixed fed-batch bioreactor has been studied using different optimization techniques, as Pontryagin Maximum Principle (see [4]), Genetic Algorithms (see [5, 6, 7, 8]) or Hybrid Stochastic-Deterministic Methods (see [4], [9]). The effects of varying the inlet flow velocity and the substrate concentration input in bioreactors have been studied as well (see for instance [10], [11], [12] and [13]). The biological purification of waste water is an example of application of bioreactors (see [14], [15] and [16]).

In this work, we consider a natural resource polluted with a substrate concentration S_{r}. The objective of the treatment is to decrease S_{r}, as fast as possible, to a target value S_{lim}, by using a bioreactor. The bioreactor is fed from the resource with a volumetric flow rate Q, and its output returns to the resource with the same flow rate Q. Typically, introducing biomass in the resource is avoided because of the risk of having bacteria growing in competition with other populations that also need oxygen. Therefore, we assume that the resource contains

only undesirable chemical substrate, that we assume to be uniformly spatially distributed all the time. To do so, the bacteria present in the bioreactor are filtered by a settler at the output so that they do not enter the resource (see Figure1).

This problem was tackled in [15] under the assumption of having a well-mixed environment, i.e., the concentration of substances were assumed homogeneous both in the water resource and in the bioreactor. Nevertheless, the activity of the bacteria inside the bioreactor induces a gradient of substrate concentration, which can be negligible or not, depending notably on the ratio between the advection and diffusion effects of the physical system. We aim at studying the influence of this gradient on the optimal inlet volumetric flow rate. Following [15], we characterize the optimal policies among constant, time-dependent and feedback controls and study the possible benefits of using non-constant flow rates. Additionally, our optimization results are compared with those obtained in [15].

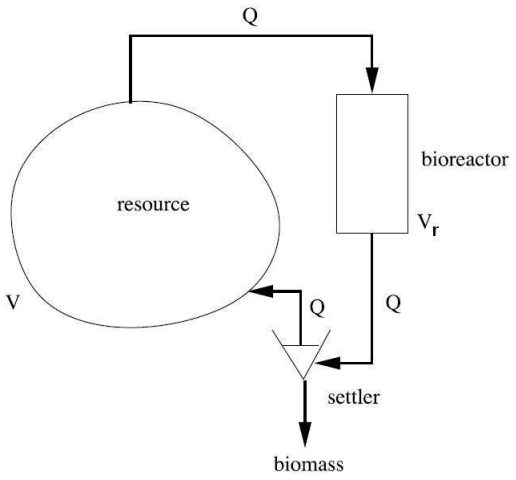


Figure 1: Connection of the bioreactor with the resource

The paper is organized as follows: Section 2 introduces an ODE model describing the behavior of the contamination in the water resource and two models describing the dynamics of the bioreactor, using ODEs and PDEs, respectively. In Section 3, we state the optimization problem, which aims to minimize the time needed to decontaminate the water resource. We also present the optimization methods used in both ODE and PDE models. In Section 4 we explain the numerical experiments carried out for the optimization problem and shows the results. Section 5 draws the conclusions after the comparison between the numerical results obtained with the ODE and PDE models.

2. Mathematical modeling

Here we detail the mathematical models used to describe the dynamics of the bioreactor and the water resource. More precisely, in Section 2.1 we present an ODE system under the assumption of uniform concentration of contaminant in the resource. We justify such an assumption for very large resource volumes for which the treatment takes long time. The output flow Q induces then a very small dilution rate of the contaminant in the resource compared to the diffusion of the contaminant, that maintains an (almost perfectly) homogeneous distribution in the resource. As the bioreactor volume is much smaller, the induced advection could make the assumption of homogeneous concentrations inside the bioreactor questionable depending on the process characteristics (reactor shape, agitation, diffusivity...). Then, in Section 2.2 we introduce two different models which describe the behavior of the concentrations inside bioreactor.

2.1. Water resource model

Since we assume homogeneous distribution of substrate in the water resource, its dynamics can be described as follows [15]:

$$\begin{cases} \frac{\mathrm{d}S_\mathrm{r}}{\mathrm{d}t} = \frac{Q}{V}(S_\mathrm{out} - S_\mathrm{r}) \qquad t > 0, \\ \\ S_\mathrm{r}(0) = S_{\mathrm{r},0}, \end{cases} \tag{1}$$

where S_r (mol/m^3) is the concentration of substrate in the water resource; V (m^3) is the water resource volume; Q (m^3/s) is the volumetric flow rate and S_out (mol/m^3) denotes the concentration of substrate concentration at the outlet of the bioreactor, which is calculated differently depending on the mathematical modeling considered for the bioreactor.
The explicit solution of (1) is

$$S_\mathrm{r}(t) = \mathrm{e}^{-\int_0^t \frac{Q(s)}{V}\mathrm{d}s} \left(\int_0^t \frac{Q(s)}{V} S_\mathrm{out}(s) \mathrm{e}^{\int_0^s \frac{Q(\tau)}{V}\mathrm{d}\tau} \mathrm{d}s + S_{\mathrm{r},0} \right). \tag{2}$$

2.2. Bioreactor Models

Section 2.2.1 presents an ODE system under the assumption of uniform concentration of substances in the bioreactor and Section 2.2.2 introduces a PDE system in order to study the influence of inhomogeneities in the tank. In both sections, $\mu(\cdot)$ (s^{-1}) denotes the growth rate function, which refers to the growth rate of the biomass in function of the substrate concentration. We assume that

$$\mu(\cdot) \text{ is increasing and concave with } \mu(0) = 0. \tag{3}$$

An example of such a growth rate function is given by the Monod equation (see, e.g., [15], [17] and [18]), which is used to relate microbial growth rates in an aqueous environment to the concentration of a limiting nutrient. Its general expression is:

$$\mu(S) = \mu_\mathrm{max} \frac{S}{K + S}, \tag{4}$$

where μ is the specific growth rate of the microorganisms, S is the concentration of limiting nutrient for growth, $\mu_{\max}$ is the maximum specific growth rate of the microorganisms and K is the *half-maximum kinetics constant*, i.e, the value of S for which $\mu(S) = \frac{\mu_{\max}}{2}$. We observe that $\mu_{\max}$ and K are empirical coefficients, that differ between species and are based on the ambient environmental conditions.

2.2.1. Homogeneous distribution in the bioreactor

We consider the following bioreactor model to describe the dynamics of the bioreactor (see [15]):

$$\begin{cases} \frac{\mathrm{d}S_{\mathrm{b}}}{\mathrm{d}t} = -\frac{\mu(S_{\mathrm{b}})B_{\mathrm{b}}}{Y} + \frac{Q}{V_{\mathrm{b}}}(S_{\mathrm{r}} - S_{\mathrm{b}}) & t > 0, \\ \frac{\mathrm{d}B_{\mathrm{b}}}{\mathrm{d}t} = \mu(S_{\mathrm{b}})B_{\mathrm{b}} - \frac{Q}{V_{\mathrm{b}}}B_{\mathrm{b}} & t > 0, \\ S_{\mathrm{b}}(0) = S_{\mathrm{b},0} \quad B_{\mathrm{b}}(0) = B_{\mathrm{b},0}, \end{cases} \tag{5}$$

where S_{b} (mol/m^3) and B_{b} (mol/m^3) denote the concentration inside the bioreactor of substrate and biomass, respectively, V_{b} (m^3) is the volume of the bioreactor and Y is a yield coefficient, which can be set to 1 without loss of generality (see for instance [18]).
If Q and S_{r} are constant, classical equilibria analysis for the bioreactor (see [18]) shows that system (5) has two equilibria, $E_1 = (S_{\mathrm{r}}, 0)$ and $E_2 = (S_{\mathrm{b}}^{\mathrm{qs}}(Q), S_{\mathrm{r}} - S_{\mathrm{b}}^{\mathrm{qs}}(Q))$, where $S_{\mathrm{b}}^{\mathrm{qs}}(Q)$ fulfills $Q = V_{\mathrm{b}}\mu(S_{\mathrm{b}}^{\mathrm{qs}}(Q))$. Moreover, E_1 is unstable and E_2 is globally asymptotically stable (excluding the case where $B_{\mathrm{b},0} = 0$) when $Q < V_{\mathrm{b}}\mu(S_{\mathrm{r}})$.

Definition 2.1. *We call washout the equilibrium state E_1, i.e., the bioreactor equilibrium with no biomass.*

A nondimensionalization analysis of systems (1) (see [19]) and (5) (see [18]) provides us with a time scale for the bioreactor, $\tau_{\mathrm{b}} = \frac{1}{\|\mu\|_\infty}$ ($\|\mu\|_\infty = \mu_{\max}$ if the Monod function (4) is considered), and for the water resource $\tau_{\mathrm{r}} = \frac{V}{V_{\mathrm{b}}}\tau_{\mathrm{b}}$. Since a reasonable hypothesis is to assume that the volume of the resource is much larger than that of the bioreactor, i.e., $V \gg V_{\mathrm{b}}$, one has that $\tau_{\mathrm{r}} \gg \tau_{\mathrm{b}}$. Thus, one can consider that the dynamics of (5) is faster than that of (1) and then make the quasi-steady state approximation, setting

$$S_{\mathrm{out}}(t) = S_{\mathrm{b}}^{\mathrm{qs}}(Q(t)) \tag{6}$$

in system (1). We point out that the hypothesis $Q(t) < V_{\mathrm{b}}\mu(S_{\mathrm{r}}(t))$ can be rewritten as $S_{\mathrm{b}}^{\mathrm{qs}}(Q(t)) \in [0, S_{\mathrm{r}}(t))$. We observe that, when $\tau_{\mathrm{r}} \gg \tau_{\mathrm{b}}$, the model given by (1),(5) is not needed and we can use (1),(6) instead.

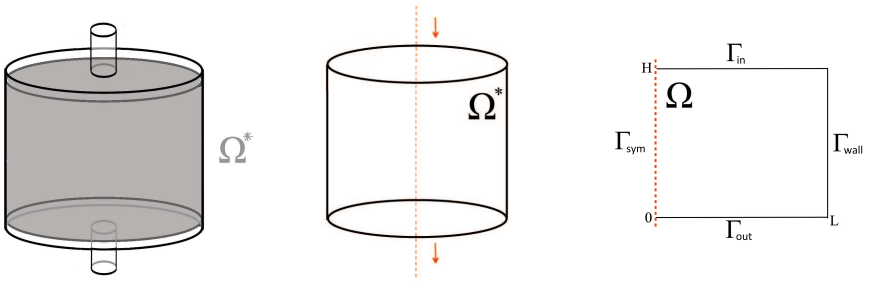
Remark 2.2. *Since the mapping $Q \to S_{\mathrm{b}}^{\mathrm{qs}}(Q)$ given by $Q = V_{\mathrm{b}}\mu(S_{\mathrm{b}}^{\mathrm{qs}}(Q))$ is a bijection from $[0, +\infty)$ to $[0, V_{\mathrm{b}}\|\mu\|_\infty)$ we will equivalently use the notations $Q = Q(S_{\mathrm{b}}^{\mathrm{qs}})$ and $S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q)$.*

2.2.2. Inhomogeneities in the bioreactor

Many works available in the literature consider non perfectly mixed bioreactors, such as tubular bioreactors with one dimensional spatialization (see for instance [20], [21], [22], [23], [24], [25]). It is of interest to consider tubular reactors with two spatial variables in order to study radial inhomogeneities of concentrations in the bioreactor. Two dimensional spatialization bioreactors are introduced, for instance, in the book of Dochain and VanRolleghem [26]. Particularly, model (2.154)-(2.159) presented in page 56, describes the behavior of the substrate and biomass concentrations in the bioreactor by using an advection-diffusion-reaction equation and a reaction equation, respectively. Moreover, Dochain and VanRolleghem consider Dankwerts boundary conditions for the substrate concentration, which are typical for continuous flow bioreactors (see, e.g., [24, 27]). Here, we modify model (2.154)-(2.159) presented in [26], by using and advection-diffusion-reaction equation together with Danckwerts boundary conditions also for the biomass.

Remark 2.3. *A typical representation of a bioreactor is a tank as depicted in Figure 2-(a), with a small inlet aperture at its top (through which polluted water enters the reactor) and a small outlet aperture at its bottom (through which the treated water leaves the reactor). In Section 2.2.2, following the model developed in [28] for fluidic mixers and for the sake of model simplification, we neglect the possible effects coming from the size and collocation of these apertures. To do that, we only model an intermediate part of the bioreactor, denoted by* Ω^* *(dark part of Figure 2-(a)), assuming that the volume of the removed part is negligible compared to the total bioreactor volume.*

Let the vertical cylinder denoted by Ω^* be the domain used for modeling the bioreactor. A typical outline of Ω^* is depicted in Figure 2-(b). At the beginning of the process, there is a certain amount of biomass inside Ω^* that reacts with the polluted water entering the reactor through the inlet Γ^*_{in} (the upper boundary of the cylinder). Treated water leaves the reactor through the outlet Γ^*_{out} (the lower boundary of the cylinder). Taking into account that the device's geometry (see



(a) 3D Reactor (b) 3D Reactor simplification (c) 2D Reactor simplification

Figure 2: Typical domain representation of the bioreactor geometry.

Figure (2)-(b)) is an empty solid of revolution, it can be simplified and described

by using a 2D domain Ω (see Figure (2)-(c)) using cylindrical coordinates. Thus, in the simplified model the domain is the rectangle $\Omega = [0, L] \times [0, H]$, where $\Gamma_{\text{sym}} = \{0\} \times (0, H)$ is the axis of symmetry; $\Gamma_{\text{in}} = (0, L) \times \{H\}$ is the bioreactor inlet; and $\Gamma_{\text{out}} = (0, L) \times \{0\}$ is the bioreactor outlet. We denote $\Gamma_{\text{wall}} = \delta\Omega \setminus (\Gamma_{\text{in}} \cup \Gamma_{\text{out}} \cup \Gamma_{\text{sym}})$, where null flux is assumed.

We consider the following advection-diffusion-reaction model to describe the dynamics in the bioreactor:

$$\begin{cases} \frac{\partial S_{\text{b}}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(rD_{\text{S}}\frac{\partial S_{\text{b}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\text{S}}\frac{\partial S_{\text{b}}}{\partial z}) - u_z\frac{\partial S_{\text{b}}}{\partial z} - \mu(S_{\text{b}})B_{\text{b}} & \text{in } (0,+\infty)\times\Omega, \\ \frac{\partial B_{\text{b}}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(rD_{\text{B}}\frac{\partial B_{\text{b}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\text{B}}\frac{\partial B_{\text{b}}}{\partial z}) - u_z\frac{\partial B_{\text{b}}}{\partial z} + \mu(S_{\text{b}})B_{\text{b}} & \text{in } (0,+\infty)\times\Omega, \\ S_{\text{b}}(0,r,z) = S_{\text{b},0} & \text{in } \Omega, \\ B_{\text{b}}(0,r,z) = B_{\text{b},0} & \text{in } \Omega, \end{cases} \tag{7}$$

where (r, z) are the cylindrical coordinates; D_{S} (m^2/s) and D_{B} (m^2/s) are the diffusion coefficients of substrate and biomass, respectively, when diffusing throughout the water in the vessel, and $\mathbf{u} = (0, u_z(t, r, z))$ is the fluid flow velocity field, where u_z (m/s) is its vertical component (radial components of the velocity field are neglected).

System (7) is completed with the following boundary conditions:

$$\begin{cases} D_{\text{S}}\frac{\partial S_{\text{b}}}{\partial z} - u_z S_{\text{b}} = -u_z S_{\text{r}}(t) & \text{on } (0,+\infty)\times\Gamma_{\text{in}}, \\ D_{\text{B}}\frac{\partial B_{\text{b}}}{\partial z} - u_z B_{\text{b}} = 0 & \text{on } (0,+\infty)\times\Gamma_{\text{in}}, \\ \frac{\partial S_{\text{b}}}{\partial r} = \frac{\partial B_{\text{b}}}{\partial r} = 0 & \text{on } (0,+\infty)\times(\Gamma_{\text{wall}}\cup\Gamma_{\text{sym}}), \\ \frac{\partial S_{\text{b}}}{\partial z} = \frac{\partial B_{\text{b}}}{\partial z} = 0 & \text{on } (0,+\infty)\times\Gamma_{\text{out}}. \end{cases} \tag{8}$$

We express the variable $S_{\text{out}}(t)$ to be used in system (1) as the substrate concentration at the outlet of the bioreactor at time t. When considering general flow velocity fields, we have to take into account that both substrate concentration and outlet flow velocity may depend on the position of the exiting particle. Thus, we considered an average value of the exiting substrate concentration weighted by the flow velocity and computed as

$$S_{\text{out}}(t) = \frac{\int_{\Gamma^*_{\text{out}}} u_z(t,x,y,0)S_{\text{b}}(t,x,y,0)\,\mathrm{d}x\mathrm{d}y}{\int_{\Gamma^*_{\text{out}}} u_z(t,x,y,0)\,\mathrm{d}x\mathrm{d}y}.$$

When expressed in cylindrical coordinates, it is calculated as

$$S_{\text{out}}(t) = \frac{\int_0^{2\pi}\int_0^L ru_z(t,r,0)S_{\text{b}}(t,r,0)\,\mathrm{d}r\mathrm{d}\theta}{\int_0^{2\pi}\int_0^L ru_z(t,r,0)\,\mathrm{d}r\mathrm{d}\theta} = \frac{\int_0^L ru_z(t,r,0)S_{\text{b}}(t,r,0)\,\mathrm{d}r}{\int_0^L ru_z(t,r,0)\,\mathrm{d}r}. \tag{9}$$

We consider two types of flow velocity fields, which do not change along the z-axis (more general fields can be considered by using the Navier-Stokes equations).

- **Homogeneous flow velocity field**: As a first approach, we consider that the vertical component of the flow velocity field is taken as $u_z(t,r,z) = u_z(t) = -Q(t)/A$, where Q (m^3/s) is the volumetric flow rate defined in Section 2.1 and A (m^2) is the area of the basis of the cylinder. In this case, $S_{\mathrm{out}}(t) = \frac{2}{L^2}\int_0^L rS_{\mathrm{b}}(t,r,0)\mathrm{d}r$.
- **Nonhomogeneous flow velocity field**: As a second approach, we consider that the flow velocity field has the shape of a paraboloid of revolution (other choices could be also considered), which is classical in Fluid Dynamics for ideal cases (see, for instance, the example given in page 41 of [29]) and more realistic than the previous homogeneous flow velocity profile. More precisely, the vertical component of the flow velocity field is taken as $u_z(t,r,z) = u_z(t,r) = -C(L^2 - r^2)$, where C is chosen so that the volume covered by half of the paraboloid of revolution is equal to Q (m^3/s). Since the volume generated is $V = C\frac{\pi}{2}L^4$, we conclude that $C(t) = \frac{2Q(t)}{\pi L^4}$ and thus $u_z(t,r) = -\frac{2Q(t)}{\pi L^4}(L^2 - r^2)$. In this case, $S_{\mathrm{out}}(t) = \frac{4}{L^4}\int_0^L r(L^2 - r^2)S_{\mathrm{b}}(t,r,0)\mathrm{d}r$.

Remark 2.4. *A nondimensionalization analysis of system (7)-(8) (see [30]) provides us with a time scale for the bioreactor, that is* $\tau_{\mathrm{b}} = \max(\frac{H^2}{D_{\mathrm{S}}}, \frac{H^2}{D_{\mathrm{B}}}, \frac{H}{u_{\max}}, \frac{1}{\|\mu\|_\infty})$, *where* $u_{\max}$ *is a suitable scale for the flow velocity component* u_z. *For the water resource, the time scale is* $\tau_{\mathrm{r}} = \frac{V}{V_{\mathrm{b}}}\frac{1}{\|\mu\|_\infty}$ *(see Section 2.2.1). For the cases where* $\tau_{\mathrm{r}} \gg \tau_{\mathrm{b}}$ *(for instance, when the volume of the resource is much larger than the volume of the bioreactor), one can consider that the dynamics of (7)-(8) is faster than that of (1), i.e, for a reasonable process time for the bioreactor, the changes in the entering substrate and the fluid flow velocity are negligible (therefore, they can be treated as constants). Consequently, when dealing with time intervals of the order of* τ_{r}, *we consider that the bioreactor is in quasi-steady state, which we approximate by taking the solution of (7)-(8) at time* t, *with* t *large enough (see [31]).*

3. Optimization problem

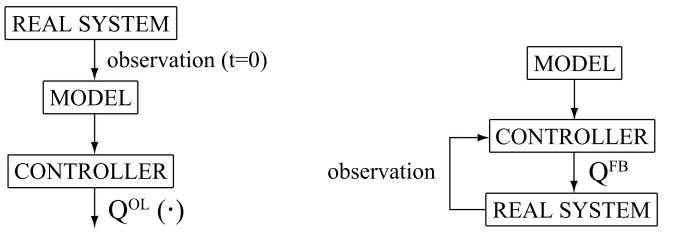
We consider the optimization problem consisting in making decrease the substrate concentration of the water resource, to a prescribed value $S_{\mathrm{lim}} > 0$ ($\mathrm{mol}/\mathrm{m}^3$), in a minimal amount of time by choosing a suitable control strategy for the input variable Q.

Definition 3.1. *We denote by* Σ_0 *and* Σ *the initial state and the state at an arbitrary time, respectively. Therefore, when considering system (1),(6)* $\Sigma_0 = S_{\mathrm{r},0}$ *and* $\Sigma = S_{\mathrm{r}} \in [0,+\infty)$; *and when considering system (1),(7)-(9) we have* $\Sigma_0 = (S_{\mathrm{r},0}, S_{\mathrm{b},0}, B_{\mathrm{b},0})$ *and* $\Sigma = (S_{\mathrm{r}}, S_{\mathrm{b}}, B_{\mathrm{b}}) \in [0,+\infty) \times (L^\infty(\Omega))^2$.

Definition 3.2.

1. *For each initial state Σ_0 we consider the set of admissible time-dependent control functions given by $\mathcal{Q}^{\mathrm{OL}} = \{Q : [0,+\infty) \to [0,+\infty)$ Lebesgue measurable such that $Q(0) < V_{\mathrm{b}}\mu(S_{\mathrm{r},0})$, where $S_{\mathrm{r},0}$ is initial state of system (1),(6) (or system (1),(7)-(9))$\}$. A functional $Q(\cdot) = Q(\Sigma_0;\cdot) \in \mathcal{Q}^{OL}$ is called an open loop-control and in the following is denoted by Q^{OL}.*
2. *We consider the set of admissible state-dependent control functions given by $\mathcal{Q}^{\mathrm{FB}} = \{Q : [0,+\infty) \to (0,+\infty)$ (resp. $Q : [0,+\infty) \times (L^{\infty}(\Omega))^2 \to [0,+\infty)$) such that system (1),(6) (resp. (1),(7)-(9)) admits a unique absolutely continuous solution for any initial condition Σ_0 and $Q(\Sigma) < V_{\mathrm{b}}\mu(S_{\mathrm{r}})\}$. A functional $Q \in \mathcal{Q}^{FB}$ is called a feedback control and in the following is denoted by Q^{FB}.* [1]

Signal flow graph representations of the two control strategies defined above are shown in Figure 3.



(a) Open-Loop control (b) Feedback control

Figure 3: Signal flow graph representations of the considered control strategies.

Remark 3.3. *The stability analysis of the ODE system (5), presented in Section 2.2.1, stated that in order to avoid washout (see Definition 2.1) a suitable condition for the flow rate Q is $Q(\Sigma) \in (0, V_{\mathrm{b}}\mu(S_{\mathrm{r}}))$. When using the ODE-PDE system (1),(7)-(9), we have presented two possible effects which may cause inhomogeneities in the bioreactor: small diffusion of substances and nonhomogeneous fluid flow velocity profile. In the first case, the entering substrate diffuses slowly through the tank and thus, smaller flow rates are needed in order to guarantee that the biomass has enough time to be in contact with the substrate and decontamination occurs. In the second case, a nonhomogeneous profile may produce that in some regions of the bioreactor, the liquid is ejected faster than if we use the homogeneous flow velocity profile, and hence, smaller flow rates are needed in order to assure that the substrate and biomass react in the whole tank. Consequently, one can conclude that the bound $Q(\Sigma) \in (0, V_{\mathrm{b}}\mu(S_{\mathrm{r}}))$ is also suitable when using the ODE-PDE system (1),(7)-(9).*

[1] The definition of $\mathcal{Q}^{FB}$ will be modified in Remark 3.6 for a special case that we will studied in this paper

Remark 3.4. *A particular case of open-loop is when Q is constant, which in the following we will be denote by Q^{C}. For each initial state Σ_0 we consider the set of admissible constant control functions given by $\mathcal{Q}^C = \{Q : [0, +\infty) \to [0, +\infty) : Q(t) = c$ for all $t \geq 0$, with $c \in [0, V_{\mathrm{b}}\mu(S_{\mathrm{lim}}))\}$.*

Remark 3.5. *For an initial state Σ_0, we call open-loop representation of the feedback Q^{FB} to the time function $Q^{\mathrm{FB}}(\cdot) = Q^{\mathrm{FB}}(\Sigma(\cdot))$ where $\Sigma(\cdot)$, is the solution of the system (either (1),(6) or (1),(7)-(9)) with initial state Σ_0.*

Remark 3.6. *For cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$, we can assume that system (1),(7)-(9) is in quasi-steady state (see Remark 2.4). In this situation, we can approximate the state of the system by $\Sigma = S_{\mathrm{r}}$ and open-loops and feedbacks can be assumed, respectively, functionals of the form $Q^{OL}(\cdot) = Q^{OL}(S_{\mathrm{r},0}; \cdot)$ and $S_{\mathrm{r}} \mapsto Q^{\mathrm{FB}}(S_{\mathrm{r}})$, where $Q^{\mathrm{FB}} \in \mathcal{Q}^{\mathrm{FB}} = \{Q : [0, +\infty) \to (0, +\infty)$ such that system (1),(7)-(9) admits a unique absolutely continuous solution for any initial condition Σ_0 and $Q(S_{\mathrm{r}}) < V_{\mathrm{b}}\mu(S_{\mathrm{r}})\}$.*

Given an initial state Σ_0, the optimization problem when using open-loops can be formulated as follows:

$$\begin{cases} \text{Find } Q^{\mathrm{OL,opt}}(\cdot) \in \mathcal{Q}^{\mathrm{OL}}, \text{ such that} \\ T(\Sigma_0, Q^{\mathrm{OL,opt}}(\cdot)) = \min\limits_{Q^{\mathrm{OL}}(\cdot) \in \mathcal{Q}^{\mathrm{OL}}} T(\Sigma_0, Q^{\mathrm{OL}}(\cdot)), \end{cases} \tag{10}$$

where $T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))$ denotes the time required to achieve $S_{\mathrm{r}}(T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))) = S_{\mathrm{lim}}$ when solving system (1),(6) (or system (1),(7)-(9)) with the flow rate $Q = Q^{\mathrm{OL}}(\cdot)$. If the target is not achieved we set $T(\Sigma_0, Q^{\mathrm{OL}}(\cdot)) = +\infty$.

The optimization problem when using feedback controls can be formulated as follows:

$$\begin{cases} \text{Find } Q^{\mathrm{FB,opt}} \in \mathcal{Q}^{\mathrm{FB}}, \text{ such that for every initial state } \Sigma_0 \\ T(\Sigma_0, Q^{\mathrm{FB,opt}}(\cdot)) = \min\limits_{Q^{\mathrm{FB}} \in \mathcal{Q}^{\mathrm{FB}}} T(\Sigma_0, Q^{\mathrm{FB}}(\cdot)), \end{cases} \tag{11}$$

where $T(\Sigma_0, Q^{FB}(\cdot))$ denotes the time required to achieve $S_{\mathrm{r}}(T(\Sigma_0, Q^{\mathrm{FB}}(\cdot))) = S_{\mathrm{lim}}$ when solving system (1),(6) (or system (1),(7)-(9)) with the flow rate $Q = Q^{\mathrm{FB}}$. If the target is not achieved we set $T(\Sigma_0, Q^{\mathrm{FB}}(\cdot)) = +\infty$.

In Section 3.1 we solve these problems considering ODE system (1),(6) and in Section 3.2 we use ODE-PDE system (1),(7)-(9).

3.1. Optimization problem with ODE system (1),(6)

When using ODE model (1),(6), we assume $\tau_{\mathrm{r}} \gg \tau_{\mathrm{b}}$. We distinguish between the cases in which Q is a constant open-loop control or a feedback control. The case where Q is a time-varying open loop is derived from the case in which Q is a feedback control (as explained in Remark 3.10).

3.1.1. Case 1: Constant open-loop control

Given an initial state $\Sigma_0 = S_{\mathrm{r},0} \in [0, +\infty)$ we look for an optimal constant $Q^{\mathrm{C,opt}} \in \mathcal{Q}^{\mathrm{C}}$ solution of (10). Under assumption (3), if control variable Q is equivalently replaced by control variable $S_{\mathrm{b}}^{\mathrm{qs}}$ (see Remark 2.2) and if we denote $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}} = \{S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q) \text{ such that } Q \in \mathcal{Q}^{\mathrm{C}}\}$, then problem (10) becomes

$$\left\{ \begin{array}{l} \text{Find } S_{\mathrm{b}}^{\mathrm{qs,C,opt}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}} \text{ such that} \\ T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C,opt}}) = \min\limits_{S_{\mathrm{b}}^{\mathrm{qs,C}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}}} T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}), \end{array} \right. \tag{12}$$

where $T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}})$ denotes the time required to achieve $S_{\mathrm{r}}(T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}})) = S_{\mathrm{lim}}$ when solving system (1),(6) with the control variable $S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs,C}}$. We now present some theoretical results that are proved in [15], about problem (12).

Lemma 3.7. *If Q is constant (i.e., $S_{\mathrm{b}}^{\mathrm{qs}}$ is constant), one has*

$$T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}) = \frac{1}{\frac{V_{\mathrm{b}}}{V}\mu(S_{\mathrm{b}}^{\mathrm{qs,C}})} \ln\left(\frac{S_{\mathrm{r},0} - S_{\mathrm{b}}^{\mathrm{qs,C}}}{S_{\mathrm{lim}} - S_{\mathrm{b}}^{\mathrm{qs,C}}}\right). \tag{13}$$

Moreover, assuming $S_{\mathrm{r},0} > S_{\mathrm{lim}}$, optimization problem (12) has a unique solution.

We approximate the solution of problem (12) by computing

$$S_{\mathrm{b}}^{\mathrm{qs,C,opt}} = \arg \min_{S_{\mathrm{b}}^{\mathrm{qs,C}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C,N}}} T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}), \tag{14}$$

where $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C,N}} = \{S_{\mathrm{b},i}^{\mathrm{qs}}\}_{i=1}^{N}$, with $N \in \mathbb{N}$ large enough and $S_{\mathrm{b},i}^{\mathrm{qs}} = \frac{i}{N+1} S_{\mathrm{lim}}$.

3.1.2. Case 2: Feedback control

In this case, we look for an optimal feedback $Q^{\mathrm{FB,opt}} \in \mathcal{Q}^{\mathrm{FB}}$ solution of (11). Under assumption (3), if control variable Q is equivalently replaced by control variable $S_{\mathrm{b}}^{\mathrm{qs}}$ and if we denote $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,FB}} = \{S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q) \text{ where } Q \in \mathcal{Q}^{\mathrm{FB}}\}$, then $S_{\mathrm{b}}^{\mathrm{qs,FB,opt}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q^{\mathrm{FB,opt}})$ is called an optimal feedback. As proven in [15], we have the following result.

Lemma 3.8. *An optimal feedback $S_{\mathrm{b}}^{\mathrm{sb,FB,opt}} : [0, +\infty) \to \mathbb{R}$ must fulfill*

$$S_{\mathrm{b}}^{\mathrm{qs,FB,opt}} = \arg \min_{S_{\mathrm{b}}^{\mathrm{qs,FB}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,FB}}} \frac{V_{\mathrm{b}}}{V} \mu(S_{\mathrm{b}}^{\mathrm{qs,FB}})(S_{\mathrm{b}}^{\mathrm{qs,FB}} - S_{\mathrm{r}}) \tag{15}$$

or, equivalently,

$$\mu'(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}})(S_{\mathrm{r}} - S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}) = \mu(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}). \tag{16}$$

Moreover, $Q^{\mathrm{FB,opt}}(\cdot)$ (see Remark 3.5) is decreasing along any optimal trajectory.

Remark 3.9. *The fact that the open loop realization of the feedback $Q^{\mathrm{FB,opt}}$ is decreasing along time can be interpreted physically as follows: as time goes on, the substrate in the water resource is decreasing and the water that enters the bioreactor is less polluted. Therefore, if $Q(\cdot)$ does not decrease, the biomass has not enough time to be in contact with the substrate in order to grow, and eventually becomes extinct.*

Remark 3.10. *If $Q^{\mathrm{FB,opt}}$ is solution of problem (11) when using system (1),(6), given an initial state $\Sigma_0 = S_{\mathrm{r},0} \in [0, +\infty)$, the open-loop representation of $Q^{\mathrm{FB,opt}}$ (see Remark 3.5) is solution of problem (10).*

3.2. Optimization problem with ODE-PDE model (1),(7)-(9)

In the case where inhomogeneities are considered, we recall that S_{out} is computed as described in (9). As in Section 3.1, we consider the cases in which Q is chosen as an open-loop control or as a feedback control.

3.2.1. Case 1: Constant open-loop control

Given an initial state $\Sigma_0 \in [0, +\infty) \times (L^\infty(\Omega))^2$ (or $\Sigma_0 \in [0, +\infty)$ for the cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$, see Remark 3.6), we look for an optimal constant $Q^{\mathrm{C,opt}} \in \mathcal{Q}^{\mathrm{C}}$ solution of problem (10), that we approximate by taking N equidistant points in the interval $(0, V_{\mathrm{b}}\mu(S_{\mathrm{lim}}))$ proceeding as in problem (14).

3.2.2. Case 2: Time varying open-loop control

Given an initial state $\Sigma_0 \in [0, +\infty) \times (L^\infty(\Omega))^2$ (or $\Sigma_0 \in [0, +\infty)$ for the cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$, see Remark 3.6), we look for a time variable function $Q^{\mathrm{OL,opt}} \in \mathcal{Q}^{\mathrm{OL}}$ close to a solution of (10). With that aim, we consider a family of time varying functions with 5 optimization parameters, denoted by Q_0, Q_1, Q_2, Q_3 and Q_4. Those optimization parameters correspond to the value of the flow rate $Q^{\mathrm{OL}}(\cdot)$ at five different given fixed times t_0, t_1, t_2, t_3 and t_4, starting from time $t_0 = 0$, so that function Q^{OL} is given by $Q^{\mathrm{OL}}(t_i) = Q_i$ $(i = 0, \ldots, 4)$, $Q^{\mathrm{OL}}(t)$ is calculated with the *monotone piecewise cubic hermite interpolation* method, with null derivatives at t_0 and t_4 (see for instance [32]) for $t \in (t_i, t_{i+1})$ $(i = 0, \ldots, 3)$, and $Q^{\mathrm{OL}}(t) = Q_4$ for $t \geq t_4$.
Following Remark 3.9, we only consider decreasing time functions $Q(\cdot)$. Thus, we compute the optimization parameters Q_0, Q_1, Q_2, Q_3 and Q_4 with the following constraints

$$Q_0 > Q_1 > Q_2 > Q_3 > Q_4.$$

To that end, we consider the optimization parameter $Q_0 \in [0, V_{\mathrm{b}}\mu(S_{\mathrm{r},0}))$ and we define new optimization parameters α_1, α_2, α_3 and α_4 in $[0, 1]$ such that the interpolation data are given by

$$Q_1 = \alpha_1 Q_0, \qquad Q_2 = \alpha_2 Q_1, \qquad Q_3 = \alpha_3 Q_2, \qquad Q_4 = \alpha_4 Q_3.$$

Therefore, we approximate $Q^{\mathrm{OL,opt}}(\cdot)$ by a function defined by interpolation, as explained above, and where the corresponding vector $\gamma^{\mathrm{opt}} = (Q_0^{\mathrm{opt}}, \alpha_1^{\mathrm{opt}}, \alpha_2^{\mathrm{opt}},$

$\alpha_3^{\rm opt}, \alpha_4^{\rm opt}$) is solution of

$$\begin{cases} \text{Find } \gamma^{\rm opt} \in (0, V_{\rm b}\mu(S_{\rm r,0})) \times (0,1)^4 \text{ such that} \\ T(\Sigma_0, Q^{\rm OL,opt}(\cdot)) = \min\limits_{\gamma \in (0, V_{\rm b}\mu(S_{\rm r,0})) \times (0,1)^4} T(\Sigma_0, Q^{\rm OL}(\cdot)), \end{cases} \tag{17}$$

where $T(\Sigma_0, Q^{\rm OL}(\cdot))$ denotes the time required to achieve $S_{\rm r}(T(\Sigma_0, Q^{\rm OL}(\cdot))) = S_{\rm lim}$ when solving (with any suitable solver; see e.g. Section 4.1) system (1) coupled with (7)-(9) with the flow rate $Q = Q^{\rm OL}(\cdot)$. We solve problem (17) with the Hybrid Genetic Algorithm (HGA), and its parameters, presented in [28]. The HGA is a global optimization algorithm based on a combination between a Genetic Algorithm (which, without requiring the computation of the gradient of the cost function, performs a first coarse global search of the solution) and a Steepest Descent method (which performs a refined local search of the solution). The suitability of this method to solve computationally expensive optimization problems has been shown in [33].

3.2.3. Case 3: Feedback Approximation

In this case, we look for an optimal feedback $Q^{\rm FB,opt} \in \mathcal{Q}^{\rm FB}$ solution of problem (11). To this end, proceeding similarly as done in Lemma 3.8 for perfectly mixed bioreactors, we perform a suboptimal strategy as a greedy policy that consists in choosing a control maximizing the instantaneous decrease of the contaminant concentration in the resource.
For cases where $\tau_{\rm b} \ll \tau_{\rm r}$, we assume that the feedback only depends on $S_{\rm r}$, i.e., $\Sigma = S_{\rm r}$ (see Remark 3.6) and we approximate the feedback function that we are looking for by solving the following optimization problem: Given an arbitrary resource substrate concentration $S \in [0, +\infty)$ and a small time interval $\Delta t > 0$ (chosen of the order of the water resource time scale $\tau_{\rm r}$ in order to assure that the bioreactor is in quasi-steady state during the time interval Δt)

$$\begin{cases} \text{Find } Q^{\rm FB,opt}(S) \in [0, V_{\rm b}\mu(S)) \text{ such that} \\ \\ S_{\rm r}(S, Q^{\rm FB,opt}; \Delta t) = \min_{Q^{\rm FB} \in [0, V_{\rm b}\mu(S))} S_{\rm r}(S, Q^{\rm FB}; \Delta t), \end{cases} \tag{18}$$

where $S_{\rm r}(S, Q^{\rm FB}; \Delta t)$ is the solution (computed with any suitable solver; see e.g Section 4.1) of system (1) coupled with (7)-(9) at time Δt, with $S = S_0$ and $Q = Q^{\rm FB}(S)$. Since $\tau_{\rm b} \ll \tau_{\rm r}$ the bioreactor is in quasi-steady state and the choice of the concentration values $S_{\rm b,0}$ and $B_{\rm b,0}$ does not have influence on the solution of problem (18). Particularly, we take $S_{\rm b,0} = B_{\rm b,0} = S$. We estimate the solution of problem (18) by taking N equidistant points in the interval $(0, V_{\rm b}\mu(S))$ and proceeding as in problem (14). Then, in order to obtain a function of the form

$$\begin{array}{rccl} Q^{\rm FB,opt}: & [S_{\rm lim}, S_{\rm r,0}] & \longrightarrow & [0, V_{\rm b}\mu(S_{\rm r,0})) \\ & S & \to & Q^{\rm FB,opt}(S), \end{array} \tag{19}$$

we solve problem (18) for a range of concentration values $S \in \mathcal{S} = \{S_i\}_{i=1}^{I+1}$, where $I \in \mathbb{N}$ is large enough and $S_i = S_{\rm r,0} - \frac{i-1}{I}(S_{\rm r,0} - S_{\rm lim})$. Finally, $Q^{\rm FB,opt}(S)$

is calculated with the *monotone piecewise cubic hermite interpolation* with null derivatives at $S_{\lim}$ and $S_{\mathrm{r},0}$ (see [32]) for $S \notin \mathcal{S}$.

For cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ is not satisfied, we approximate the feedback function that we are looking for by solving the following optimization problem: Given arbitrary concentration values $(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \in [0, +\infty) \times (L^\infty(\Omega))^2$ and a small time interval $\Delta t > 0$

$$\begin{cases} \text{Find } Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \in [0, V_{\mathrm{b}}\mu(S)) \text{ such that} \\ \\ S_{\mathrm{r}}(\Sigma, Q^{\mathrm{FB,opt}}; \Delta t) = \min_{Q^{\mathrm{FB}} \in [0, V_{\mathrm{b}}\mu(S))} S_{\mathrm{r}}(S, Q^{\mathrm{FB}}; \Delta t), \end{cases} \tag{20}$$

where $S_{\mathrm{r}}(S, Q^{\mathrm{FB}}; \Delta t)$ is the solution (obtained with a suitable numerical solver; see e.g. Section 4.1) of system (1) coupled with (7)-(9) at time Δt, with $\Sigma_0 = (S, s_{\mathrm{b}}, b_{\mathrm{b}})$ and $Q = Q^{\mathrm{FB}}(S, s_{\mathrm{b}}, b_{\mathrm{b}})$. We estimate the solution of problem (20) by taking N equidistant points in the interval $(0, V_{\mathrm{b}}\mu(S))$ and proceeding as in problem (14).
Then, in order to obtain a function of the form

$$\begin{array}{rccc} Q^{\mathrm{FB,opt}}: & [S_{\lim}, S_{\mathrm{r},0}] \times (L^\infty(\Omega))^2 & \longrightarrow & [0, V_{\mathrm{b}}\mu(S_{\mathrm{r},0})) \\ & (S, s_{\mathrm{b}}, b_{\mathrm{b}}) & \to & Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}}), \end{array} \tag{21}$$

we solve problem (20) for a range of concentration values $(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ in the set $\mathcal{M} = \{(S, s_{\mathrm{b}}, b_{\mathrm{b}}) : \exists i \in \{1, \dots, I+1\}$ such that $S = S_i \in \mathcal{S}$, $s_{\mathrm{b}} \in \mathcal{S}_{\mathrm{b},i}$ and $b_{\mathrm{b}} \in \mathcal{B}_{\mathrm{b},i}\}$ where $S_i = S_{\mathrm{r},0} - \frac{i-1}{I}(S_{\mathrm{r},0} - S_{\lim})$, $\mathcal{S}_{\mathrm{b},i} = \mathcal{B}_{\mathrm{b},i} = \{S_{i,j}\}_{j \in J}$ with $J \subset \mathbb{N}$ and $S_{i,j} = \frac{S_i}{j}$. If $(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \notin \mathcal{M}$, we compute the mean value of the concentrations s_{b} and b_{b} in the bioreactor (which we denote by $\overline{s}_{\mathrm{b}}$ and $\overline{b}_{\mathrm{b}}$) by

$$\overline{s}_{\mathrm{b}} = \frac{2\displaystyle\int_0^L \int_0^H r s_{\mathrm{b}}(r, z)\, \mathrm{d}z\mathrm{d}r}{L^2 H}, \quad \overline{b}_{\mathrm{b}} = \frac{2\displaystyle\int_0^L \int_0^H r b_{\mathrm{b}}(r, z)\, \mathrm{d}z\mathrm{d}r}{L^2 H},$$

and $Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ is approximated by $Q^{\mathrm{FB,opt}}(S, \overline{s}_{\mathrm{b}}, \overline{b}_{\mathrm{b}})$, which is given by *spatial interpolation*. More specifically, $Q^{\mathrm{FB,opt}}(S, \overline{s}_{\mathrm{b}}, \overline{b}_{\mathrm{b}})$ is calculated with a suitable *trilinear* or *neighbor interpolation* method depending if $(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ is or not inside the convex hull of $\mathcal{M}$.

Remark 3.11. *Solution of problems (18) and (20) are approximations of the solution of problem (11) which, as shown in Section 4.3, provide satisfactory results.*

4. Numerical Experiments

In this section, we first introduce the numerical solvers used for computing the solutions of systems (1),(6) and (1),(7)-(9). Then, in Sections 4.2 and 4.3 we present the numerical results obtained when looking for constant and feedback controls, respectively. Notice that in order to shorten the presentation of this work, the results obtained when looking for time varying open-loop controls has been included in Section 4.3.

4.1. Numerical solvers used for systems (1),(6) and (1),(7)-(9)

The solution of system (1),(6) was computed numerically by using a fourth-order Runge-Kutta method and the solution of system (1),(7)-(9) was computed numerically by coupling a fourth-order Runge-Kutta method with a Finite Element Method (see [34]). The computational experiments were carried out with a 2.8Ghz Intel i7-930 64bits computer with 12Gb of RAM. We used a triangular mesh with around 600 elements. A numerical simulation of system (1),(7)-(9) with time step $\Delta t = 100$s and final time 10^5s, computed using MATLAB (`mathworks.com`) and COMSOL Multyphisics 5.0 (`www.comsol.com`), takes approximately 12 seconds.

Model parameters were taken following [15, 35]: $\mu(\cdot)$ was the Monod Function (see (4)) with $\mu_{\max} = 1$ (s^{-1}) and $K = 1$ (mol/m^3). For the bioreactor and water resource volumes we took $V_b = 1$ (m^3) and $V = 1000$ (m^3), respectively. In order to obtain a cylinder of volume $V_b = 1$ (m^3), we used a 2D bioreactor domain with $H = L = 0.68$ (m). We considered a case for which the time scale of the bioreactor was comparable to the time scale of the water resource by using diffusion coefficients $D_S = D_B = 0.01$ (m^2/s). We also consider a case where the time scale for the bioreactor was much smaller than the time scale of the water resource by using diffusion coefficients $D_S = D_B = 100$ (m^2/s). When computing a constant open loop control (see Section 3.2.1), $N = 100$ was chosen to solve problem (14). When computing a time-varying open loop (see Section 3.2.2), the interpolation times were $t_0 = 0$ (s), $t_1 = 20000$(s), $t_2 = 40000$(s), $t_3 = 60000$(s) and $t_4 = 80000$(s). Those values where taken equidistant and having estimated experimentally that the time needed to achieve the prescribed value in the resource is around 10^5s. Finally, when computing a feedback (see Section 3.2.3), problems (18) and (20) were solved by using the MATLAB functions `interp1` and `interp3` (see `https://www.mathworks.com/moler/interp.pdf`), respectively, with $\Delta t = 100$ s.

Remark 4.1. *The model parameters considered here were chosen as in [15] in order to obtain a straightforward comparison between the methodologies proposed in this article and the ones introduced here. Of course, they could be replaced by other values found in the literature.*

4.2. Constant Open-Loop Control

In this Section, we solve numerically the optimization problem (10) when the volumetric flow rate Q is considered a constant. More specifically, Section 4.2.1 shows the numerical results for the ODE system (1),(6), obtained by solving problem (14), and Section 4.2.2 shows the numerical results for the ODE-PDE system (1),(7)-(9), obtained as explained in Section 3.2.1. Then, in Section 4.2.3 we make a comparison of the results obtained in Sections 4.2.1 and 4.2.2 in terms of the optimal constant open-loop controls and the time needed to achieve the prescribed value of substrate concentration in the water resource, $S_{\lim}$. We also compare systems (1),(6) and (1),(7)-(9) in terms of the minimum substrate concentration achieved in the water resource if the constant flow rate

obtained for system (1),(6) is used in system (1),(7)-(9). Simulations were done with initial substrate concentration in the resource $S_{\mathrm{r},0} = 10$ (mol/m^3) and with $S_{\mathrm{lim}} = 0.1$ (mol/m^3). These simulations were also performed for $S_{\mathrm{r},0} = 5$ (mol/m^3) and similar conclusions were obtained.

4.2.1. ODE system (1),(6)

In this Section we solve the optimization problem (14) using system (1),(6) with $N = 200$. The optimal constant open-loop is $Q_{\mathrm{ODE}}^{\mathrm{C,opt}} = 0.0790$ (m^3/s) and the corresponding decontamination time is $T(S_{\mathrm{r},0}, Q_{\mathrm{ODE}}^{\mathrm{C,opt}}) = 81830$ (s).

4.2.2. ODE-PDE model (1),(7)-(9)

In this Section we solve the optimization problem (10) using the model given by system (1),(7)-(9). We denote $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ the optimal constant flow rates when considering the homogeneous and the nonhomogeneous flow velocity fields, respectively. Equivalently, we denote $S_{\mathrm{r,ach}}^{\mathrm{H}}$ and $S_{\mathrm{r,ach}}^{\mathrm{NH}}$ the minimum substrates concentrations achieved in the water resource if $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in system (1),(7)-(9). For these concentration values, the flow rate $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is high enough to drive system (1),(7)-(9) to washout (see Definition 2.1), i.e., the biomass become extinct and no more reaction is produced.

We distinguish between the cases where the time scale of the bioreactor is much smaller than the time scale of the water resource (i.e., $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$) and the case where that condition is not satisfied.

- **Case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$:**
  Table 1 shows optimal constant open loops and the corresponding decontamination times. The substrate concentrations achieved in the resource are $S_{\mathrm{r,ach}}^{\mathrm{H}} = 0.08569$ (mol/m^3) and $S_{\mathrm{r,ach}}^{\mathrm{NH}} = 0.1177$ (mol/m^3).

$S_{\mathrm{r},0}$ (mol/m^3)	$Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{H}}^{\mathrm{C,opt}})$ (s)	$Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{NH}}^{\mathrm{C,opt}})$ (s)
10	0.0778	81840	0.0594	110420

Table 1: ODE-PDE model: case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$. Values of the optimal constant open-loops $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the corresponding decontamination times for $S_{\mathrm{r},0} = 10$ (mol/m^3).

- **Case $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$:**
  In this case, the optimal constant open loop also depends on the initial state at the bioreactor. Since we aim to compare the optimal constant open-loop controls obtained for the ODE system (1),(6) and the ODE-PDE system (1),(7)-(9), we estimate a function of the form $S_{\mathrm{r},0} \to Q_{\mathrm{H}}^{\mathrm{C,opt}}(S_{\mathrm{r},0})$ by solving problem (10) for a range of initial states in the set $\mathcal{M}$ defined to solve problem (20) with $I = 1$ and $J = \{1, 2, 4, 10\}$. Then, $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ is approximated by computing the mean value of the set of optimal constant open-loop controls obtained for the different initial states.

This procedure is also used to obtain the optimal constant $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the substrate concentrations $S_{\mathrm{r,ach}}^{\mathrm{H}}$ and $S_{\mathrm{r,ach}}^{\mathrm{NH}}$.
Table 2 shows the optimal constant flow rates and the corresponding decontamination times. The substrate concentrations achieved in the resource are $S_{\mathrm{r,ach}}^{\mathrm{H}} = 0.1524$ (mol/m^3) and $S_{\mathrm{r,ach}}^{\mathrm{NH}} = 0.1776$ (mol/m^3).

$S_{\mathrm{r},0}$ (mol/m^3)	$Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{H}}^{\mathrm{C,opt}})$ (s)	$Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{NH}}^{\mathrm{C,opt}})$ (s)
10	0.0547	102190	0.0442	129160

Table 2: ODE-PDE model: case $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$. Values of the optimal constant open-loops $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the corresponding decontamination times for $S_{\mathrm{r},0} = 10$ (mol/m^3).

4.2.3. Discussion

An interesting study is to check if the optimization results obtained in Sections 4.2.1 and 4.2.2 are similar. We make the comparison for both flow velocity fields, described in Section 2.2.2.

- **Homogenous flow velocity field**: We can observe from results in Section 4.2.1 and Table 1 that the volumetric flow rates $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (obtained with the ODE-PDE system (1),(7)-(9) when $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$) are significantly close and the decontamination times are comparable (the difference is below 1% for both values of $S_{\mathrm{r},0}$). Nevertheless, from results in Section 4.2.1 and Table 2 one notice that the flow rate $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (obtained with the ODE-PDE system (1),(7)-(9) when $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$) is around 70% of the value of $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$. Furthermore, from the value $S_{\mathrm{r,ach}}^{\mathrm{H}}$ we conclude that if the constant $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is applied in system (1),(7)-(9) in the case where $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$, the bioreactor is driven to washout (see Definition 2.1) before the decontamination target is achieved. These results seem to indicate that when high diffusions are considered, the optimal constant controls obtained with the ODE model are similar to those obtained with the ODE-PDE model, whereas for low diffusion coefficients the ODE-PDE model exhibits better results, in the sense that it provides smaller volumetric flow rates which favor that the biomass does not become extinct in the bioreactor before the target is achieved (see Remark 3.3).

- **Nonhomogeneous flow velocity field**: We can observe from results in Section 4.2.1 and Tables 1 and 2 that the volumetric flow rates $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$, obtained with the ODE-PDE system (1),(7)-(9) in the cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ and $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$, are around 75% and 60% of the value of the flow rate $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$, respectively. Furthermore, from the values $S_{\mathrm{r,ach}}^{\mathrm{NH}}$ we conclude that if the constant $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in the ODE-PDE system (1),(7)-(9), the bioreactor is driven to washout (see Definition 2.1) before the decontamination target

is achieved. These results seem to indicate that when the nonhomogeneous flow velocity field is considered, model (1),(7)-(9) exhibits better results, in the sense that it provides smaller volumetric flow rates which favor that the biomass does not become extinct in the bioreactor before the target is achieved (see Remark 3.3).

4.3. Feedback

In this Section, we look for an optimal feedback, denoted by $Q^{\mathrm{FB,opt}}$ solution of problem (11). More specifically, Section 4.3.1 shows the results for the ODE system (1),(6), obtained using Lemma 3.8 and Section 4.3.2 shows the feedback approximations for the ODE-PDE system (1),(7)-(9), obtained when solving the suboptimal problems (18) and (20). Section 4.3.2 also shows the feedback synthesis (see definition below) of the optimal time varying open-loops, obtained when solving (17). Then, in Section 4.3.3 we make a comparison of the results presented in Sections 4.3.1 and 4.3.2 in terms of the feedback control. Furthermore, we compare models (1),(6) and (1),(7)-(9) in terms of the minimum substrate concentration achieved in the water resource if the optimal feedback obtained for system (1),(6) is used in system (1),(7)-(9).

4.3.1. ODE model (1),(6)

As detailed in Section 3.1.2 if the Monod equation (4) is taken, the optimal feedback, denoted by $Q^{\mathrm{FB,opt}}_{\mathrm{ODE}}$, fulfills

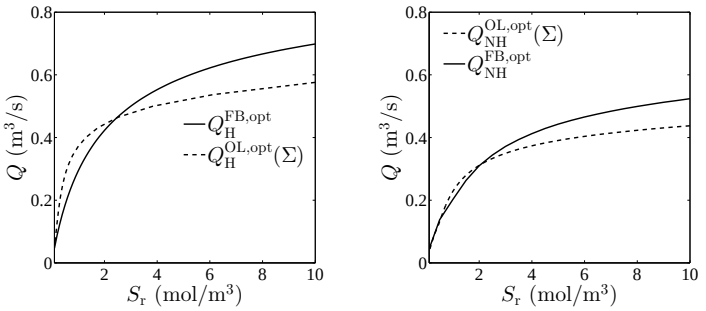
$$Q^{\mathrm{FB,opt}}_{\mathrm{ODE}} = V_{\mathrm{b}}\mu(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}) = V_{\mathrm{b}}\mu(\sqrt{K^2 + K \cdot S_{\mathrm{r}}} - K).$$

4.3.2. ODE-PDE model (1),(7)-(9)

As a first approach, we solve problem (11) by solving optimization problems (18) and (20) (considering a feedback approximation, as described in Section 3.2.3), for both homogeneous and nonhomogeneous flow velocity fields, denoting the solution by $Q^{\mathrm{FB,opt}}_{\mathrm{H}}$ and $Q^{\mathrm{FB,opt}}_{\mathrm{NH}}$, respectively.
In order to compare with time varying open-loop controls (see Section 3.2.2), as a second approach we solve problem (11) by solving the optimization problem (17) and then taking the feedback synthesis of the time varying open-loop, i.e., for any time t with corresponding values $Q(t)$ and $\Sigma(t)$, we can reconstruct the map $\Sigma(t) \to Q(t)$, that can be seen as a state-dependent control function, which in the following we denote by $Q^{\mathrm{OL,opt}}_{\mathrm{H}}(\Sigma)$ and $Q^{\mathrm{OL,opt}}_{\mathrm{NH}}(\Sigma)$, for the homogeneous and the nonhomogeneous flow velocity fields, respectively. Equivalently, we denote $S^{\mathrm{H}}_{\mathrm{r,ach}}$ and $S^{\mathrm{NH}}_{\mathrm{r,ach}}$ the minimum substrate concentrations achieved in the water resource if $Q^{\mathrm{FB,opt}}_{\mathrm{ODE}}$ is used in system (1),(7)-(9). For these concentration value, the flow rate $Q^{\mathrm{ODE}}_{\mathrm{FB,opt}}$ is high enough to drive system (1),(7)-(9) to washout (see Definition 2.1), i.e., the biomass become extinct and no more reaction is produced.

Simulations have been conducted for substrate concentration $S_{\mathrm{r},0} = 10$ (mol/m^3) $S_{\mathrm{lim}} = 0.1$ (mol/m^3).

- **Case** $\tau_{\rm b} \ll \tau_{\rm r}$
  Figure 4 shows the similarities between the feedbacks obtained with the two approaches described above. More precisely, Figure 4-(a) shows the feedbacks $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm H}^{\rm OL,opt}(\Sigma)$ and Figure4-(b) shows the feedbacks $Q_{\rm NH}^{\rm FB,opt}$ and $Q_{\rm NH}^{\rm OL,opt}(\Sigma)$, while the corresponding decontamination times are shown in Table 3. Note that, for the sake of comparison, Table 3 also includes the decontamination times $T(S_{\rm r,0}, Q_{\rm ODE}^{\rm C,opt})$, obtained in Section 4.2.1.



(a) Homogeneous flow velocity field (b) Nonhomogeneous flow velocity field

Figure 4: ODE-PDE model: case $\tau_{\rm b} \ll \tau_{\rm r}$. Comparison between the feedback approximations $Q^{\rm FB,opt}$ (depicted with solid lines) and $Q^{\rm OL,opt}$ (depicted with dashed lines).

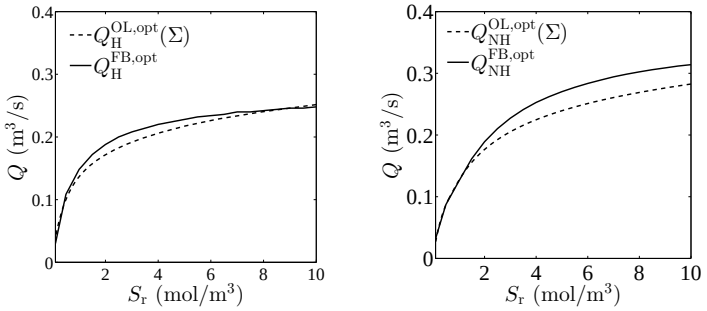
$T(S_{\rm r,0}, Q_{\rm H}^{\rm FB,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm H}^{\rm OL,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm H}^{\rm C,opt})$ (s)
49870	48040	81840
$T(S_{\rm r,0}, Q_{\rm NH}^{\rm FB,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm NH}^{\rm OL,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm NH}^{\rm C,opt})$ (s)
64770	63990	110420

Table 3: ODE-PDE model: case $\tau_{\rm b} \ll \tau_{\rm r}$. Decontamination times obtained with system (1),(7)-(9), $S_{\rm r,0} = 10$ (mol/m^3) and controls $Q^{\rm FB,opt}$, $Q^{\rm OL,opt}$ and $Q^{\rm C,opt}$.

- **Case** $\tau_{\rm b} \approx \tau_{\rm r}$:
  In this case, time varying open loops and feedbacks depend on the bioreactor state. Since we aim to compare the optimal feedback obtained for ODE model (1),(6) with the two feedback schemes obtained for ODE-PDE model (1),(7)-(9), we approximate functions of the form $S_{\rm r} \to Q_{\rm H}^{\rm FB,opt}(S_{\rm r})$ and $S_{\rm r,0} \to Q_{\rm H}^{\rm OL,opt}(S_{\rm r,0};\cdot)$. In order to compute $Q_{\rm H}^{\rm FB,opt}(S_{\rm r})$ (or $Q_{\rm NH}^{\rm FB,opt}(S_{\rm r})$) we solve problem (20) for $(S, s_{\rm b}, b_{\rm b})$ in the set $\mathcal{M}$, defined to solve problem (18), with $I = 20$ and $J = \{1, 2, 4, 10\}$. Thus, for each $S \in \mathcal{S}$, $Q^{\rm FB,opt}(S)$ is approximated by computing the mean value of the set of optimal feedbacks $Q^{\rm FB,opt}(S, s_{\rm b}, b_{\rm b})$ with $(S, s_{\rm b}, b_{\rm b}) \in \mathcal{M}$. Similarly, in order to compute $Q_{\rm H}^{\rm OL,opt}(S_{\rm r,0};\cdot)$ we solve problem (17), taking $\Sigma_0 \in \mathcal{M}$

with $I = 1$ and $J = \{1, 2, 4, 10\}$. Then, each component of vector γ^{opt} is approximated by computing the mean value of the set of its optimal values obtained for the different initial states. This procedure is also used to obtain the average optimal time varying open loop $Q_{\text{NH}}^{\text{C,opt}}(S_{\text{r,0}};\cdot)$ and substrate concentrations $S_{\text{r,ach}}^{\text{H}}$ and $S_{\text{r,ach}}^{\text{NH}}$.

Figure 5 shows the similarities between the feedbacks obtained with the two approaches described above. More precisely, Figure 5-(a) shows the feedbacks $Q_{\text{H}}^{\text{FB,opt}}$ and $Q_{\text{H}}^{\text{OL,opt}}(\Sigma)$, obtained when considering the homogeneous flow velocity field. Figure 5-(b) shows the feedbacks $Q_{\text{NH}}^{\text{FB,opt}}$ and $Q_{\text{NH}}^{\text{OL,opt}}(\Sigma)$, obtained when considering the nonhomogeneous flow velocity field. The corresponding decontamination times are shown in Table 4. Note that, for the sake of comparison, Table 4 also includes the decontamination times $T(S_{\text{r,0}}, Q_{\text{ODE}}^{\text{C,opt}})$, obtained in Section 4.2.1. The substrate concentrations achieved in the resource are $S_{\text{r,ach}}^{\text{H}} = 9.9888$ (mol/m^3) and $S_{\text{r,ach}}^{\text{NH}} = 9.9836$ (mol/m^3).



(a) Homogeneous flow velocity field (b) Nonhomogeneous flow velocity field

Figure 5: ODE-PDE model: Case $\tau_{\text{b}} \approx \tau_{\text{r}}$. Comparison between the feedback approximations $Q^{\text{FB,opt}}$ (depicted with solid lines) and $Q^{\text{OL,opt}}(\Sigma)$ (depicted with dashed lines).

$T(S_{\text{r,0}}, Q_{\text{H}}^{\text{FB,opt}})$ (s)	$T(S_{\text{r,0}}, Q_{\text{H}}^{\text{OL,opt}})$ (s)	$T(S_{\text{r,0}}, Q_{\text{H}}^{\text{C,opt}})$ (s)
58900	57610	102190
$T(S_{\text{r,0}}, Q_{\text{NH}}^{\text{FB,opt}})$ (s)	$T(S_{\text{r,0}}, Q_{\text{NH}}^{\text{OL,opt}})$ (s)	$T(S_{\text{r,0}}, Q_{\text{NH}}^{\text{C,opt}})$ (s)
74050	74180	129160

Table 4: ODE-PDE model: case $\tau_{\text{b}} \ll \tau_{\text{r}}$. Decontamination times obtained with system (1),(7)-(9), $S_{\text{r,0}} = 10$ (mol/m^3) and controls $Q^{\text{FB,opt}}$, $Q^{\text{OL,opt}}$ and $Q^{\text{C,opt}}$.

4.3.3. Discussion

An interesting study is to check if both approaches, described in Sections 3.2.2 and 3.2.3, present similar numerical results. From Figure 4 and Figure 5

one can observe significant similarities between the two volumetric flow rates $Q^{\mathrm{FB,opt}}$ and $Q^{\mathrm{OL,opt}}(\Sigma)$, being the first one a bit faster than the second one in most of the cases. This result is not surprising, since the open-loop approach takes into account the concentrations only at initial time, while the feedback strategy is intrinsically more robust.

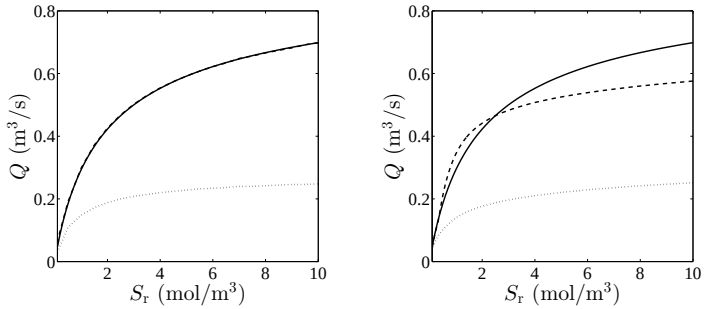
Another interesting study is to check if the optimization results obtained in Sections 4.3.1 and 4.3.2 are similar. We make the comparison for both flow velocity profiles, described in Section 2.2.2.

- **Homogenous flow velocity field**: In order to analyze the similarities between the obtained optimal controls $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$, $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$, we plot them in Figure 6. It is easy to observe that the volumetric flow rates $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$ (obtained with the ODE-PDE system (1),(7)-(9) in the case where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$) are significantly close to the flow rate $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ (in fact, $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ seem indistinguishable in Figure 6-(a)). Nevertheless, the flow rates $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$ (obtained with the ODE-PDE system (1),(7)-(9) when $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$) are much slower than $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$. For instance, for $S_{\mathrm{r}} = 10$ (mol/m^3) the values of $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$ are around 35% the value of $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$. Furthermore, from the value $S_{\mathrm{r,ach}}^{\mathrm{H}}$, we conclude that if the constant control $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ is used in system (1),(7)-(9) the bioreactor is driven to washout (see Definition 2.1) before the decontamination target is achieved. These results seem to show that when high diffusions are considered, the optimal controls obtained with the ODE and ODE-PDE models are similar, whereas for low diffusion coefficients the ODE-PDE model exhibits better results, in the sense that it provides smaller volumetric flow rates that favor that the biomass does not become extinct before the target is achieved.

- **Nonhomogeneous flow velocity field**: In order to analyze the similarities between the obtained optimal controls $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$, $Q_{\mathrm{NH}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{OL,opt}}(\Sigma)$, we plot them in Figure 7. It is easy to observe that the volumetric flow rates $Q_{\mathrm{NH}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{OL,opt}}(\Sigma)$, obtained with the ODE-PDE system (1),(7)-(9) when $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ and $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$, are respectively around 75% and 35% the value of the flux $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$. As a result we can conclude that the ODE-PDE systems exhibits better results when computing the optimal feedback, in the sense that it provides smaller volumetric flow rates that favor that the biomass does not become extinct before the target is achieved.

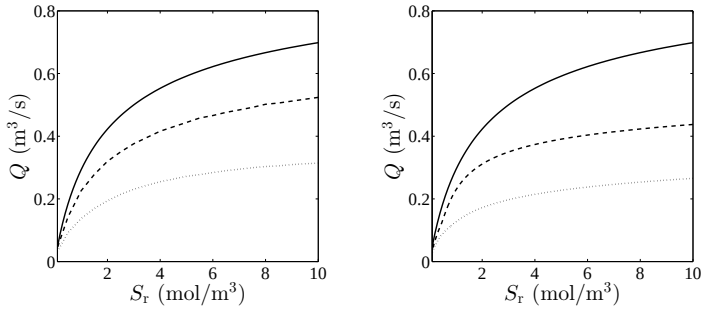
Comparison between the considered control strategies

Here, we compare the open-loop and feedback controls obtained in Sections 4.2.2 and 4.3.2. From Tables 3 and 4, one can observe that the decontamination times obtained using time-varying open loops and feedbacks are similar.



(a) $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ vs $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ (b) $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ vs $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$

Figure 6: Homogeneous flow velocity field: Comparison between the feedback obtained for the ODE model (depicted with solid line), the feedback obtained for the ODE-PDE model when $\tau_\mathrm{b} \ll \tau_\mathrm{r}$ (depicted with dashed lines) and the feedback obtained for the ODE-PDE model when $\tau_\mathrm{b} \approx \tau_\mathrm{r}$ (depicted with dotted lines).



(a) $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ vs $Q_{\mathrm{NH}}^{\mathrm{FB,opt}}$ (b) $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ vs $Q_{\mathrm{NH}}^{\mathrm{OL,opt}}(\Sigma)$

Figure 7: Nonhomogeneous flow velocity field: Comparison between the feedback obtained for the ODE model (depicted with solid line), the feedback obtained for the ODE-PDE model when $\tau_\mathrm{b} \ll \tau_\mathrm{b}$(depicted with dashed lines) and the feedback obtained for the ODE-PDE model when $\tau_\mathrm{b} \approx \tau_\mathrm{r}$ (depicted with dotted lines).

However, the feedback approximation exhibits two advantages with respect to the time-dependent control: it is more robust to possible changes on the system conditions and, once obtained, it can be applied in other scenarios without additional computational cost. Finally, one can see that the decontamination times among constant controls are twice larger than those among time-varying open loops and feedbacks.

5. Conclusion

In this work, we have focused on the modeling of the problem of water treatment by using continuous bioreactors. We have presented two mathematical models, assuming homogeneity or inhomogeneity of substrate and biomass

concentrations in the bioreactor. We have also made a difference between considering that the fluid flow velocity in the bioreactor is homogeneous through the inlet, or follows a nonhomogeneous profile.

We have tackled an optimization problem which aims to minimize the time needed to clean the polluted resource, by choosing an optimal bioreactor volumetric inflow rate. In the case of considering homogeneity of the contaminant in the bioreactor, it is possible to obtain analytically an optimal flow rate from previous theoretical results. In the case of considering inhomogeneity of the contaminant in the bioreactor, we show here how to obtain an optimal flow rate using an hybrid genetic algorithm. The results show that, in the cases where the time scale in the bioreactor is comparable with the time scale of the resource (for instance, by using $D_{\mathrm{S}} = D_{\mathrm{B}} = 0.01$ $(\mathrm{m}^2/\mathrm{s})$), the optimal flow rates are smaller than the optimal flow rates obtained for the mathematical model which considers homogeneity in the bioreactor. In any case, the decontamination time can be substantially reduced if feedback controls are used instead of constant controls.

Our goal was to compare the numerical optimization results obtained for the ODE and ODE-PDE models presented for coupled system between the bioreactor and the water resource. The results show that when the time scale of the bioreactor is much smaller than the one of the water resource, (for instance, by using $D_{\mathrm{S}} = D_{\mathrm{B}} = 100$ $(\mathrm{m}^2/\mathrm{s})$), the ODE-PDE system with homogeneous flow velocity field approaches the ODE system. Contrarily, the ODE-PDE system with nonhomogeneous flow velocity field does not approach the ODE system in the sense that, when using the control strategy that is optimal under the homogeneous assumption in the bioreactor, the biomass becomes extinct and it is not able to make the substrate in the water resource decrease to the objective value. Let us notice that the nonhomogeneous flow velocity field has been presented in order to approach a more realistically behavior of the reactor (see [29]). An important conclusion is that an optimal feedback derived for perfectly mixed bioreactor can lead a bioreactor with non negligible diffusion terms to washout, preventing the desired decontamination objective to be reached, while a simple open loop control, obtained with the method presented in this work, can solve the problem.

Acknowledgements

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Modeling and optimization of activated sludge bioreactors for wastewater treatment taking into account spatial inhomogeneities

M. Crespo[a,b,c,*], B. Ivorra[a], A.M. Ramos[a], A. Rapaport[b]

[a] *Departamento de Matemática Aplicada & Instituto de Matemática Interisciplinar, Universidad Complutense de Madrid. Plaza de Ciencias, 3, 28040 Madrid, Spain.*
[b] *UMR MISTEA - Mathématiques,Informatique et Statistique pour l´ Environnement et l´ Agronomie (INRA/SupAgro). 2, Place P.Viala, 34060 Montpellier, France.*
[c] *Université Montpellier, Labex Numev. 161, rue Ada, 34095 Montpellier Cedex 5, France.*

Abstract

In this work, we study optimal and suboptimal control strategies for the treatment of a polluted water resource by using aside a continuous bioreactor. The control consists in choosing the inlet volumetric flow rate for filling the bioreactor with contaminated water from a considered resource (lake, reservoir, water-table...). The treated outflow returns to the resource. We tackle an optimization problem which aims to minimize the time needed to reach a prescribed minimal value of contamination in the resource by choosing the input flow. Next, we study the influence of inhomogeneities of concentrations in the bioreactor, considering a system based on partial differential equations which describe its dynamics. We show that applying the optimal feedback control derived for perfectly mixed bioreactor does not allow to reach the target with small diffusion parameters as it drives the bioreactor to washout (the bioreactor equilibrium with no biomass). In this case, a suboptimal feedback (which reaches the target in finite time) is obtained with the help of a Hybrid Genetic Algorithm. Furthermore, we consider that the fluid flow velocity of the water entering into the bioreactor follows either a uniform or a nonuniform profile, showing that the optimal volumetric flow rates obtained with the uniform profile are not optimal if the profile is nonuniform, even when high diffusion coefficients are considered in the model.

Keywords: water treatment, bioreactor, advection diffusion reaction model, optimal control

*Corresponding author
Email addresses: mcresp01@ucm.es (M. Crespo), ivorra@mat.ucm.es (B. Ivorra), angel@mat.ucm.es (A.M. Ramos), alain.rapaport@umr.fr (A. Rapaport)

1. Introduction

The decontamination of water resources is a major environmental issue in the areas of prevention of eutrophication and wastewater treatment. Eutrophication is a process whereby water resources becomes too rich in organic material and mineral nutrients. Household products (phosphorus detergents) and products used in agriculture (nitrate fertilizers) are the main causes of pollution of water resources. As a result, some plants (in particular planktonic algae) can grow rapidly and reduce the available oxygen of the aquatic ecosystem resulting, for instance, in the death of local bio-organisms (such as fishes). The *activated sludge process* is a way of eliminating eutrophication from water resources. The process uses biomass (i.e., bacteria) to feed with substrate (i.e., the organic contaminant) in wastewater, producing a high quality effluent for a reasonable operating and maintenance cost. It consists of several interrelated components:

- A tank where the biological reaction occurs, called bioreactor. Bacteria thrive as they travel through the bioreactor and they multiply rapidly with sufficient food (substrate).
- A waste water source that feeds the bioreactor.
- A settler situated at the bottom of the bioreactor, separating bacteria from the clearer water. This accumulated bacteria is called *activated sludge*.
- A means of collecting the activated sludge, either to return it to the bioreactor or to remove it from the process.

~~Three modes of operation are very common in activated sludge bioreactor execution: batch, continuous and fed-batch. During batch operation no substrate is added to the initial charge and the product is not removed until the end of the process; in continuous operation the substrate is continually added and product continually removed; in fed-batch operation the feed rate may be changed during the process, but no product is removed until the end. One of the advantages of the continuous mode regarding batch and fed-batch (see [1, 2]), is that it does not require necessarily upstream tanks (i.e., tanks used to stock contaminated water that cannot be treated immediately by the bioreactor).~~

The optimization of activated sludge processes has received a great attention in the literature (see, e.g.,[3], [4] and [5] for reviews of the different optimization techniques that have been used in bioprocesses). The objective is usually to control the inlet flow rate of the bioreactor for attaining a prescribed target (e.g., a small prescribed amount of pollutant at the bioreactor outlet) in a finite given time. Particularly, the maximization of bacteria production in a well mixed fed-batch bioreactor has been studied using different optimization techniques, as Pontryagin Maximum Principle (see [6]), Genetic Algorithms (see [7, 8, 9, 10]) or Hybrid Stochastic-Deterministic Methods (see [6], [11]). The effects of varying the inlet flow velocity and the substrate concentration input in ~~continuous~~ bioreactors have been studied as well (see for instance [12], [13], [14] and [15]). The biological purification of waste water is an example of application

of ~~continuous~~ bioreactors (see [16], [17] and [18]). ~~Specifically, the influence of inhomogeneity was studied in~~ [17] [19] [20]~~, where the problem of water treatment was tackled when considering non homogeneous substrate concentration in the water resource.~~

~~Typically, introducing biomass in the resource is forbidden because of the risk of having bacteria growing in competition with other populations that also need oxygen. Therefore, we assume that the resource contains only undesirable chemical substrate, that we assume to be distributed uniformly all the time. Bacteria are present only in the bioreactor and filtered by a settler at the output so that they do not enter the resource. The activity of the bacteria inside the bioreactor induces a gradient of substrate concentration, which can be negligible or not, depending on the ratio between the advection and diffusion effects of the physical system. We aim at studying the influence of this gradient on the optimal inlet volumetric flow rate. Following~~ [17]~~, we consider a natural resource polluted with a substrate concentration S_r. The objective of the treatment is to decrease S_r, as fast as possible, to a target value S_{lim}, by using a bioreactor. The bioreactor is fed from the resource with a volumetric flow rate Q, and its output returns to the resource with the same flow rate Q (we implicitly assume that the impact of the volume of the collected biomass on the flow rate is negligible), after separation of biomass in a settler (See Figure~~ 1).

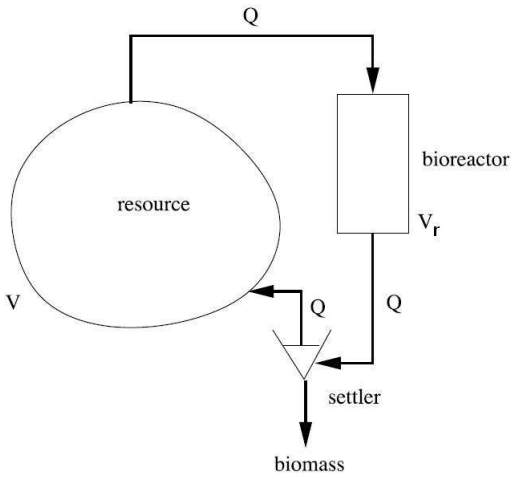


Figure 1: Connection of the bioreactor with the resource

In this work, we consider a natural resource polluted with a substrate concentration S_r. The objective of the treatment is to decrease S_r, as fast as possible, to a target value S_{lim}, with the help of a bioreactor. The bioreactor is fed from the resource with a volumetric flow rate Q, and its output returns to the resource with the same flow rate Q. Typically, introducing biomass in the

resource is avoided because of the risk of having bacteria growing in competition with other populations that also need oxygen. Therefore, we assume that the resource contains only undesirable chemical substrate, that we assume to be uniformly spatially distributed all the time. To do so, the bacteria present in the bioreactor are filtered by a settler at the output so that they do not enter the resource (see Figure1).

This problem was tackled in [17] under the assumption of having a well-mixed environment, i.e., the concentration of substances were assumed homogeneous both in the water resource and in the bioreactor. Nevertheless, the activity of the bacteria inside the bioreactor induces a gradient of substrate concentration, which can be negligible or not, depending notably on the ratio between the advection and diffusion effects of the physical system. We aim at studying the influence of this gradient on the optimal inlet volumetric flow rate control problem. Following [17], we characterize the optimal policies among constant, time-dependent and feedback controls and study the possible benefits of using non-constant flow rates. Additionally, our optimization results are compared with those obtained in [17].

The paper is organized as follows: Section 2 introduces an ODE model describing the behavior of the contamination in the water resource and two models describing the dynamics of the bioreactor, using ODEs and PDEs, respectively. In Section 3, we state the optimization problem, which aims to minimize the time needed to decontaminate the water resource. We also present the optimization methods used in both ODE and PDE models. In Section 4 we explain the numerical experiments carried out for the optimization problem and shows the results. Section 5 draws the conclusions after the comparison between the numerical results obtained with the ODE and PDE models.

2. Mathematical modeling

Here we detail the mathematical models used to describe the dynamics of the bioreactor and the water resource. More precisely, in Section 2.1 we present an ODE system under the assumption of uniform concentration of contaminant in the resource. We justify such an assumption for very large resource volumes for which the treatment takes long time. The output flow Q induces then a very small dilution rate of the contaminant in the resource compared to the diffusion of the contaminant, that maintains an (almost perfectly) homogeneous distribution in the resource. As the bioreactor volume is much smaller, the induced advection could make the assumption of homogeneous concentrations inside the bioreactor questionable depending on the process characteristics (reactor shape, agitation, diffusivity...). Then, in Section 2.2 we introduce two different models which describe the behavior of the concentrations inside bioreactor.

2.1. Water resource model

Since we assume homogeneous distribution of substrate in the water resource, its dynamics can be described as follows [17]:

$$\begin{cases} \frac{\mathrm{d}S_\mathrm{r}}{\mathrm{d}t} = \frac{Q}{V}(S_\mathrm{out} - S_\mathrm{r}) \qquad t > 0, \\ \\ S_\mathrm{r}(0) = S_{\mathrm{r},0}, \end{cases} \tag{1}$$

where S_r (mol/m^3) is the concentration of substrate in the water resource; V (m^3) is the water resource volume; Q (m^3/s) is the volumetric flow rate and S_out (mol/m^3) denotes the concentration of substrate concentration at the outlet of the bioreactor, which is calculated differently depending on the mathematical modeling considered for the bioreactor.
The explicit solution of (1) is

$$S_\mathrm{r}(t) = \mathrm{e}^{-\int_0^t \frac{Q(s)}{V}\mathrm{d}s} \left(\int_0^t \frac{Q(s)}{V} S_\mathrm{out}(s) \mathrm{e}^{\int_0^s \frac{Q(\tau)}{V}\mathrm{d}\tau} \mathrm{d}s + S_{\mathrm{r},0} \right). \tag{2}$$

2.2. Bioreactor Models

Section 2.2.1 presents an ODE system under the assumption of uniform concentration of substances in the bioreactor and Section 2.2.2 introduces a PDE system in order to study the influence of inhomogeneities in the tank. In both sections, $\mu(\cdot)$ (s^{-1}) denotes the growth rate function, which refers to the growth rate of the biomass in function of the substrate concentration. We assume that

$$\mu(\cdot) \text{ is increasing and concave with } \mu(0) = 0. \tag{3}$$

An example of such a growth rate function is given by the Monod equation (see, e.g., [17], [21] and [22]), which is used to relate microbial growth rates in an aqueous environment to the concentration of a limiting nutrient. Its general expression is:

$$\mu(S) = \mu_\mathrm{max} \frac{S}{K + S}, \tag{4}$$

where μ is the specific growth rate of the microorganisms, S is the concentration of limiting nutrient for growth, μ_max is the maximum specific growth rate of the microorganisms and K is the *half-maximum kinetics constant*, i.e, the value of S for which $\mu(S) = \frac{\mu_\mathrm{max}}{2}$. We observe that μ_max and K are empirical coefficients, that differ between species and are based on the ambient environmental conditions.

2.2.1. Homogeneous distribution in the bioreactor

We consider the following bioreactor model to describe the dynamics of the bioreactor (see [17]):

$$\begin{cases} \frac{\mathrm{d}S_\mathrm{b}}{\mathrm{d}t} = -\frac{\mu(S_\mathrm{b})B_\mathrm{b}}{Y} + \frac{Q}{V_\mathrm{b}}(S_\mathrm{r} - S_\mathrm{b}) \qquad t > 0, \\ \\ \frac{\mathrm{d}B_\mathrm{b}}{\mathrm{d}t} = \mu(S_\mathrm{b})B_\mathrm{b} - \frac{Q}{V_\mathrm{b}}B_\mathrm{b} \qquad\qquad t > 0, \\ \\ S_\mathrm{b}(0) = S_{\mathrm{b},0} \quad B_\mathrm{b}(0) = B_{\mathrm{b},0}, \end{cases} \tag{5}$$

where S_b (mol/m^3) and B_b (mol/m^3) denote the concentration inside the bioreactor of substrate and biomass, respectively, V_b (m^3) is the volume of the bioreactor and Y is a yield coefficient, which can be set to 1 without loss of generality (see for instance [22]).
If Q and S_r are constant, classical equilibria analysis for the bioreactor (see [22]) shows that system (5) has two equilibria, $E_1 = (S_\mathrm{r}, 0)$ and $E_2 = (S_\mathrm{b}^\mathrm{qs}(Q), S_\mathrm{r} - S_\mathrm{b}^\mathrm{qs}(Q))$, where $S_\mathrm{b}^\mathrm{qs}(Q)$ fulfills $Q = V_\mathrm{b}\mu(S_\mathrm{b}^\mathrm{qs}(Q))$. Moreover, E_1 is unstable and E_2 is globally asymptotically stable (excluding the case where $B_{\mathrm{b},0} = 0$) when $Q < V_\mathrm{b}\mu(S_\mathrm{r})$.

Definition 2.1. *We call washout the equilibrium state E_1, i.e., the bioreactor equilibrium with no biomass.*

A nondimensionalization analysis of systems (1) (see [23]) and (5) (see [22]) provides us with a time scale for the bioreactor, $\tau_\mathrm{b} = \frac{1}{\|\mu\|_\infty}$ ($\|\mu\|_\infty = \mu_\mathrm{max}$ if the Monod function (4) is considered), and for the water resource $\tau_\mathrm{r} = \frac{V}{V_\mathrm{b}}\tau_\mathrm{b}$. Since a reasonable hypothesis is to assume that the volume of the resource is much larger than that of the bioreactor, i.e., $V \gg V_\mathrm{b}$, one has that $\tau_\mathrm{r} \gg \tau_\mathrm{b}$. Thus, one can consider that the dynamics of (5) is faster than that of (1) and then make the quasi-steady state approximation, setting

$$S_\mathrm{out}(t) = S_\mathrm{b}^\mathrm{qs}(Q(t)) \tag{6}$$

in system (1). We point out that the hypothesis $Q(t) < V_\mathrm{b}\mu(S_\mathrm{r}(t))$ can be rewritten as $S_\mathrm{b}^\mathrm{qs}(Q(t)) \in [0, S_\mathrm{r}(t))$. We observe that, when $\tau_\mathrm{r} \gg \tau_\mathrm{b}$, the model given by (1),(5) is not needed and we can use (1),(6) instead. ~~Furthermore, according to (2), when Q is constant the explicit solution of system (1),(6) is given by~~

~~$$S_\mathrm{r}(t) = S_\mathrm{b}^\mathrm{qs}(Q) + (S_{\mathrm{r},0} - S_\mathrm{b}^\mathrm{qs}(Q))\mathrm{e}^{-\frac{V_\mathrm{b}}{V}\mu(S_\mathrm{b}^\mathrm{qs}(Q))t}.$$~~ (7)

Remark 2.2. *Since the mapping $Q \to S_\mathrm{b}^\mathrm{qs}(Q)$ given by $Q = V_\mathrm{b}\mu(S_\mathrm{b}^\mathrm{qs}(Q))$ is a bijection from $[0, +\infty)$ to $[0, V_\mathrm{b}\|\mu\|_\infty)$, ~~we can use as the ODE model for the water resource~~*

~~$$\begin{cases} \frac{\mathrm{d}S_\mathrm{r}}{\mathrm{d}t}(t) = \frac{Q}{V}(\mu^{-1}(\frac{Q}{V_\mathrm{b}}) - S_\mathrm{r}(t)) \qquad t > 0, \\ S_\mathrm{r}(0) = S_{\mathrm{r},0}, \end{cases}$$~~ (8)

~~*or, equivalently*~~

~~$$\begin{cases} \frac{\mathrm{d}S_\mathrm{r}}{\mathrm{d}t}(t) = \frac{V_\mathrm{b}}{V}\mu(S_\mathrm{b}^\mathrm{qs})(S_\mathrm{b}^\mathrm{qs} - S_\mathrm{r}(t)) \qquad t > 0, \\ S_\mathrm{r}(0) = S_{\mathrm{r},0}. \end{cases}$$~~ (9)

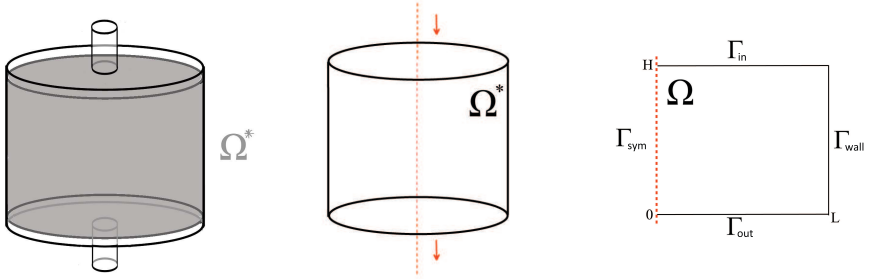
~~*Due to the bijection mentioned above,*~~ *we will equivalently use the notations $Q = Q(S_\mathrm{b}^\mathrm{qs})$ and $S_\mathrm{b}^\mathrm{qs} = S_\mathrm{b}^\mathrm{qs}(Q)$.* ~~*Giving a function S_b^qs is equivalent to give a function Q, and viceversa.*~~

2.2.2. Inhomogeneities in the bioreactor

Many works available in the literature consider non perfectly mixed bioreactors, such as tubular bioreactors with one dimensional spatialization (see for instance [24], [25], [26], [27], [28], [29]). It is of interest to consider tubular reactors with two spatial variables in order to study radial inhomogeneities of concentrations in the bioreactor. Two dimensional spatialization bioreactors are introduced, for instance, in the book of Dochain and VanRolleghem [30]. Particularly, model (2.154)-(2.159) presented in page 56, describes the behavior of the substrate and biomass concentrations in the bioreactor by using an advection-diffusion-reaction equation and a reaction equation, respectively. Moreover, Dochain and VanRolleghem consider Dankwerts boundary conditions for the substrate concentration, which are typical for continuous flow bioreactors (see, e.g., [28, 31]). Here, we modify model (2.154)-(2.159) presented in [30], by using and advection-diffusion-reaction equation together with Danckwerts boundary conditions also for the biomass.

Remark 2.3. *A typical representation of a bioreactor is a tank as depicted in Figure 2-(a), with a small inlet aperture at its top (through which polluted water enters the reactor) and a small outlet aperture at its bottom (through which the treated water leaves the reactor). In Section 2.2.2, following the model developed in [32] for fluidic mixers and for the sake of model simplification, we neglect the possible effects coming from the size and collocation of these apertures. To do that, we only model an intermediate part of the bioreactor, denoted by* Ω^* *(dark part of Figure 2-(a)), assuming that the volume of the removed part is negligible compared to the total bioreactor volume.*

Let the vertical cylinder denoted by Ω^* be the domain used for modeling the bioreactor. A typical outline of Ω^* is depicted in Figure 2-(b). At the beginning of the process, there is a certain amount of biomass inside Ω^* that reacts with the polluted water entering the reactor through the inlet Γ^*_{in} (the upper boundary of the cylinder). Treated water leaves the reactor through the outlet Γ^*_{out} (the lower boundary of the cylinder). Taking into account that the device's geometry (see



(a) 3D Reactor (b) 3D Reactor simplification (c) 2D Reactor simplification

Figure 2: Typical domain representation of the bioreactor geometry.

Figure (2)-(b)) is an empty solid of revolution, it can be simplified and described

by using a 2D domain Ω (see Figure (2)-(c)) using cylindrical coordinates. Thus, in the simplified model the domain is the rectangle $\Omega = [0, L] \times [0, H]$, where $\Gamma_{\text{sym}} = \{0\} \times (0, H)$ is the axis of symmetry; $\Gamma_{\text{in}} = (0, L) \times \{H\}$ is the bioreactor inlet; and $\Gamma_{\text{out}} = (0, L) \times \{0\}$ is the bioreactor outlet. We denote $\Gamma_{\text{wall}} = \delta\Omega \setminus (\Gamma_{\text{in}} \cup \Gamma_{\text{out}} \cup \Gamma_{\text{sym}})$, where null flux is assumed.

We consider the following advection-diffusion-reaction model to describe the dynamics in the bioreactor:

$$\begin{cases} \frac{\partial S_{\text{b}}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(rD_{\text{S}}\frac{\partial S_{\text{b}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\text{S}}\frac{\partial S_{\text{b}}}{\partial z}) - u_z\frac{\partial S_{\text{b}}}{\partial z} - \mu(S_{\text{b}})B_{\text{b}} & \text{in } (0,+\infty)\times\Omega, \\ \frac{\partial B_{\text{b}}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(rD_{\text{B}}\frac{\partial B_{\text{b}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\text{B}}\frac{\partial B_{\text{b}}}{\partial z}) - u_z\frac{\partial B_{\text{b}}}{\partial z} + \mu(S_{\text{b}})B_{\text{b}} & \text{in } (0,+\infty)\times\Omega, \\ S_{\text{b}}(0,r,z) = S_{\text{b},0} & \text{in } \Omega, \\ B_{\text{b}}(0,r,z) = B_{\text{b},0} & \text{in } \Omega, \end{cases} \tag{10}$$

where (r, z) are the cylindrical coordinates; D_{S} (m^2/s) and D_{B} (m^2/s) are the diffusion coefficients of substrate and biomass, respectively, when diffusing throughout the water in the vessel, and $\mathbf{u} = (0, u_z(t, r, z))$ is the fluid flow velocity field, where u_z (m/s) is its vertical component (radial components of the velocity field are neglected).

System (10) is completed with the following boundary conditions:

$$\begin{cases} D_{\text{S}}\frac{\partial S_{\text{b}}}{\partial z} - u_z S_{\text{b}} = -u_z S_{\text{r}}(t) & \text{on } (0,+\infty)\times\Gamma_{\text{in}}, \\ D_{\text{B}}\frac{\partial B_{\text{b}}}{\partial z} - u_z B_{\text{b}} = 0 & \text{on } (0,+\infty)\times\Gamma_{\text{in}}, \\ \frac{\partial S_{\text{b}}}{\partial r} = \frac{\partial B_{\text{b}}}{\partial r} = 0 & \text{on } (0,+\infty)\times(\Gamma_{\text{wall}}\cup\Gamma_{\text{sym}}), \\ \frac{\partial S_{\text{b}}}{\partial z} = \frac{\partial B_{\text{b}}}{\partial z} = 0 & \text{on } (0,+\infty)\times\Gamma_{\text{out}}. \end{cases} \tag{11}$$

Remark 2.4. ~~*If $S_{\text{b},0} \geq 0$ in Ω, $S_{\text{b},0}$, $B_{\text{b},0} \in L^\infty(\Omega)$, $S_{\text{r}} \in L^\infty(0,\infty)$, μ is lipschitz, $\mu(0) = 0$ and $\mu(z) \geq 0$ for $z \geq 0$, then system (10)-(11) has a unique solution $(S_{\text{b}}, B_{\text{b}}) \in (\mathcal{C}([0,+\infty); L^2(\Omega)) \cap L^\infty((0,\infty)\times\Omega))^2$ (see [33]).*~~

We express the variable $S_{\text{out}}(t)$ to be used in system (1) as the substrate concentration at the outlet of the bioreactor at time t. When considering general flow velocity fields, we have to take into account that both substrate concentration and outlet flow velocity may depend on the position of the exiting particle. Thus, we considered an average value of the exiting substrate concentration weighted by the flow velocity and computed as

$$S_{\text{out}}(t) = \frac{\int_{\Gamma^*_{\text{out}}} u_z(t,x,y,0) S_{\text{b}}(t,x,y,0)\,\text{d}x\text{d}y}{\int_{\Gamma^*_{\text{out}}} u_z(t,x,y,0)\,\text{d}x\text{d}y}.$$

When expressed in cylindrical coordinates, it is calculated as

$$S_{\text{out}}(t) = \frac{\int_0^{2\pi}\int_0^L r u_z(t,r,0) S_{\text{b}}(t,r,0)\,\mathrm{d}r\mathrm{d}\theta}{\int_0^{2\pi}\int_0^L r u_z(t,r,0)\,\mathrm{d}r\mathrm{d}\theta} = \frac{\int_0^L r u_z(t,r,0) S_{\text{b}}(t,r,0)\,\mathrm{d}r}{\int_0^L r u_z(t,r,0)\,\mathrm{d}r}. \quad (12)$$

We consider two types of flow velocity fields, which do not change along the z-axis (more general fields can be considered by using the Navier-Stokes equations).

- **Homogeneous flow velocity field**: As a first approach, we consider that the vertical component of the flow velocity field is taken as $u_z(t,r,z) = u_z(t) = -Q(t)/A$, where Q (m^3/s) is the volumetric flow rate defined in Section 2.1 and A (m^2) is the area of the basis of the cylinder. In this case, $S_{\text{out}}(t) = \frac{2}{L^2}\int_0^L r S_{\text{b}}(t,r,0)\mathrm{d}r$.
- **Nonhomogeneous flow velocity field**: As a second approach, we consider that the flow velocity field has the shape of a paraboloid of revolution (other choices could be also considered), which is classical in Fluid Dynamics for ideal cases (see, for instance, the example given in page 41 of [34]) and more realistic than the previous homogeneous flow velocity profile. More precisely, the vertical component of the flow velocity field is taken as $u_z(t,r,z) = u_z(t,r) = -C(L^2 - r^2)$, where C is chosen so that the volume covered by half of the paraboloid of revolution is equal to Q (m^3/s). Since the volume generated is $V = C\frac{\pi}{2}L^4$, we conclude that $C(t) = \frac{2Q(t)}{\pi L^4}$ and thus $u_z(t,r) = -\frac{2Q(t)}{\pi L^4}(L^2 - r^2)$. In this case, $S_{\text{out}}(t) = \frac{4}{L^4}\int_0^L r(L^2 - r^2) S_{\text{b}}(t,r,0)\mathrm{d}r$.

Remark 2.5. *A nondimensionalization analysis of system (10)-(11) (see [35]) provides us with a time scale for the bioreactor, that is* $\tau_{\text{b}} = \max(\frac{H^2}{D_{\text{S}}}, \frac{H^2}{D_{\text{B}}}, \frac{H}{u_{\max}}, \frac{1}{\|\mu\|_\infty})$, *where* $u_{\max}$ *is a suitable scale for the flow velocity component* u_z. *For the water resource, the time scale is* $\tau_{\text{r}} = \frac{V}{V_{\text{b}}}\frac{1}{\|\mu\|_\infty}$ *(see Section 2.2.1). For the cases where* $\tau_{\text{r}} \gg \tau_{\text{b}}$ *(for instance, when the volume of the resource is much larger than the volume of the bioreactor), one can consider that the dynamics of (10)-(11) is faster than that of (1), i.e, for a reasonable process time for the bioreactor, the changes in the entering substrate and the fluid flow velocity are negligible (therefore, they can be treated as constants). Consequently, when dealing with time intervals of the order of* τ_{r}, *we consider that the bioreactor is in quasi-steady state, which we approximate by taking the solution of (10)-(11) at time* t, *with* t *large enough (see [36]).*

~~*Under this hypothesis, system (10)-(11) can be changed, at each time* $t \in (0, +\infty)$,~~

~~by~~

$$\begin{cases} \frac{1}{r}\frac{\partial}{\partial r}(rD_{\mathrm{S}}\frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\mathrm{S}}\frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial z}) - u_z\frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} = \mu(S_{\mathrm{b}}^{\mathrm{qs}})B_{\mathrm{b}}^{\mathrm{qs}} & \text{in } \Omega, \\ \frac{1}{r}\frac{\partial}{\partial r}(rD_{\mathrm{B}}\frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial r}) + \frac{\partial}{\partial z}(D_{\mathrm{B}}\frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial z}) - u_z\frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} = -\mu(S_{\mathrm{b}}^{\mathrm{qs}})B_{\mathrm{b}}^{\mathrm{qs}} & \text{in } \Omega, \\ D_{\mathrm{S}}\frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} - u_z S_{\mathrm{b}}^{\mathrm{qs}} = -u_z S_{\mathrm{r}} & \text{on } \Gamma_{\mathrm{in}}, \\ D_{\mathrm{B}}\frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} - u_z B_{\mathrm{b}}^{\mathrm{qs}} = 0 & \text{on } \Gamma_{\mathrm{in}}, \\ \frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial r} = \frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial r} = 0 & \text{on } \Gamma_{\mathrm{wall}} \cup \Gamma_{\mathrm{sym}}, \\ \frac{\partial S_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} = \frac{\partial B_{\mathrm{b}}^{\mathrm{qs}}}{\partial z} = 0 & \text{on } \Gamma_{\mathrm{out}}, \end{cases} \tag{13}$$

~~*where $u_z(t,\cdot)$ and $S_{\mathrm{r}}(t)$ are time dependent and $(S_{\mathrm{b}}^{\mathrm{qs}}(t,r,z), B_{\mathrm{b}}^{\mathrm{qs}}(t,r,z))$ (mol/m^3) are the substrate and biomass concentrations of the bioreactor in quasi-steady state, respectively. A usual way to solve numerically nonlinear system (13) is to solve numerically (10)-(11) (which is usually easier) and then take the solution corresponding to large values of t as the solution of (13) (see [36]). Therefore, computing numerically the solution of system (13) could be very heavy. This is why in the following we consider and solve system (1),(10)-(12), also for the cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$.*~~

3. Optimization problem

We consider the optimization problem consisting in making decrease the substrate concentration of the water resource, to a prescribed value $S_{\mathrm{lim}} > 0$ (mol/m^3), in a minimal amount of time by choosing a suitable control strategy for the input variable Q.

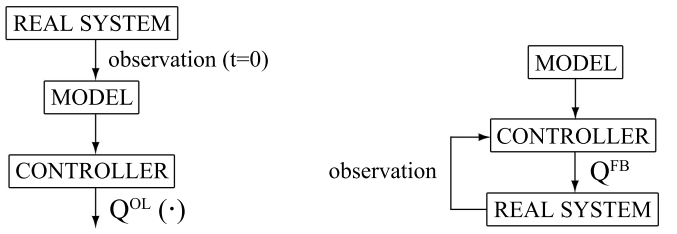
Definition 3.1. *We denote by Σ_0 and Σ the initial state and the state at an arbitrary time, respectively. Therefore, when considering system (1),(6) $\Sigma_0 = S_{\mathrm{r},0}$ and $\Sigma = S_{\mathrm{r}} \in [0,+\infty)$; and when considering system (1),(10)-(12) we have $\Sigma_0 = (S_{\mathrm{r},0}, S_{\mathrm{b},0}, B_{\mathrm{b},0})$ and $\Sigma = (S_{\mathrm{r}}, S_{\mathrm{b}}, B_{\mathrm{b}}) \in [0,+\infty) \times (L^\infty(\Omega))^2$.*

Definition 3.2.

1. *For each initial state Σ_0 we consider the set of admissible time-dependent control functions given by $\mathcal{Q}^{\mathrm{OL}} = \{Q : [0,+\infty) \to [0,+\infty)$ Lebesgue measurable such that $Q(0) < V_{\mathrm{b}}\mu(S_{\mathrm{r},0})$, where $S_{\mathrm{r},0}$ is initial state of system (1),(6) (or system (1),(10)-(12))$\}$. A functional $Q(\cdot) = Q(\Sigma_0;\cdot) \in \mathcal{Q}^{OL}$ is called an open loop-control and in the following is denoted by Q^{OL}.*
2. *We consider the set of admissible state-dependent control functions given by $\mathcal{Q}^{\mathrm{FB}} = \{Q : [0,+\infty) \to (0,+\infty)$ (resp. $Q : [0,+\infty) \times (L^\infty(\Omega))^2 \to [0,+\infty)$) such that system (1),(6) (resp. (1),(10)-(12)) admits a unique absolutely continuous solution for any initial condition Σ_0 and $Q(\Sigma) <$*

$V_b\mu(S_r)\}$. *A functional* $Q \in \mathcal{Q}^{FB}$ *is called a feedback control and in the following is denoted by* Q^{FB}. [1]

Signal flow graph representations of the two control strategies defined above are shown in Figure 3.



(a) Open-Loop control (b) Feedback control

Figure 3: Signal flow graph representations of the considered control strategies.

Remark 3.3. *The stability analysis of the ODE system (5), presented in Section 2.2.1, stated that in order to avoid washout (see Definition 2.1) a suitable condition for the flow rate* Q *is* $Q(\Sigma) \in (0, V_b\mu(S_r))$. *When using the ODE-PDE system (1),(10)-(12), we have presented two possible effects which may cause inhomogeneities in the bioreactor: small diffusion of substances and non-homogeneous fluid flow velocity profile. In the first case, the entering substrate diffuses slowly through the tank and thus, smaller flow rates are needed in order to guarantee that the biomass has enough time to be in contact with the substrate and decontamination occurs. In the second case, a nonhomogeneous profile may produce that in some regions of the bioreactor, the liquid is ejected faster than if we use the homogeneous flow velocity profile, and hence, smaller flow rates are needed in order to assure that the substrate and biomass react in the whole tank ~~(see Remark 4.2 for better explanation of the second case)~~. Consequently, one can conclude that the bound* $Q(\Sigma) \in (0, V_b\mu(S_r))$ *is also suitable when using the ODE-PDE system (1),(10)-(12).*

Remark 3.4. *A particular case of open-loop is when* Q *is constant, which in the following we will be denote by* Q^C. *For each initial state* Σ_0 *we consider the set of admissible constant control functions given by* ~~$\mathcal{Q}^C = \{Q : [0, +\infty) \to [0, +\infty)$: $Q(t) \equiv c$ with $c \in [0, V_b\mu(S_{r,0}))\}$. Furthermore, since the objective is to decrease the substrate concentration of the water resource to a prescribed value S_{lim} in minimal time, the set of admissible constant control functions is reduced to~~ $\mathcal{Q}^C = \{Q : [0, +\infty) \to [0, +\infty) : Q(t) = c$ *for all* $t \geq 0$, *with* $c \in [0, V_b\mu(S_{lim}))\}$.

[1] The definition of $\mathcal{Q}^{FB}$ will be modified in Remark 3.6 for a special case that we will studied in this paper

Remark 3.5. *For an initial state Σ_0, we call open-loop representation of the feedback Q^{FB} to the time function $Q^{\mathrm{FB}}(\cdot) = Q^{\mathrm{FB}}(\Sigma(\cdot))$ where $\Sigma(\cdot)$, is the solution of the system (either (1),(6) or (1),(10)-(12)) with initial state Σ_0.*

Remark 3.6. *For cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$, we can assume that system (1),(10)-(12) is in quasi-steady state (see Remark 2.5). In this situation, we can approximate the state of the system by $\Sigma = S_{\mathrm{r}}$ and open-loops and feedbacks can be assumed, respectively, functionals of the form $Q^{OL}(\cdot) = Q^{OL}(S_{\mathrm{r},0}; \cdot)$ and $S_{\mathrm{r}} \mapsto Q^{\mathrm{FB}}(S_{\mathrm{r}})$, where $Q^{\mathrm{FB}} \in \mathcal{Q}^{\mathrm{FB}} = \{Q : [0, +\infty) \to (0, +\infty)$ such that system (1),(10)-(12) admits a unique absolutely continuous solution for any initial condition Σ_0 and $Q(S_{\mathrm{r}}) < V_{\mathrm{b}}\mu(S_{\mathrm{r}})\}$.*

Given an initial state Σ_0, the optimization problem when using open-loops can be formulated as follows:

$$\begin{cases} \text{Find } Q^{\mathrm{OL,opt}}(\cdot) \in \mathcal{Q}^{\mathrm{OL}}, \text{ such that} \\ T(\Sigma_0, Q^{\mathrm{OL,opt}}(\cdot)) = \min\limits_{Q^{\mathrm{OL}}(\cdot) \in \mathcal{Q}^{\mathrm{OL}}} T(\Sigma_0, Q^{\mathrm{OL}}(\cdot)), \end{cases} \tag{14}$$

where $T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))$ denotes the time required to achieve $S_{\mathrm{r}}(T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))) = S_{\mathrm{lim}}$ when solving system (1),(6) (or system (1),(10)-(12)) with the flow rate $Q = Q^{\mathrm{OL}}(\cdot)$. If the target is not achieved we set $T(\Sigma_0, Q^{\mathrm{OL}}(\cdot)) = +\infty$.

The optimization problem when using feedback controls can be formulated as follows:

$$\begin{cases} \text{Find } Q^{\mathrm{FB,opt}} \in \mathcal{Q}^{\mathrm{FB}}, \text{ such that for every initial state } \Sigma_0 \\ T(\Sigma_0, Q^{\mathrm{FB,opt}}(\cdot)) = \min\limits_{Q^{\mathrm{FB}} \in \mathcal{Q}^{\mathrm{FB}}} T(\Sigma_0, Q^{\mathrm{FB}}(\cdot)), \end{cases} \tag{15}$$

where $T(\Sigma_0, Q^{FB}(\cdot))$ denotes the time required to achieve $S_{\mathrm{r}}(T(\Sigma_0, Q^{\mathrm{FB}}(\cdot))) = S_{\mathrm{lim}}$ when solving system (1),(6) (or system (1),(10)-(12)) with the flow rate $Q = Q^{\mathrm{FB}}$. If the target is not achieved we set $T(\Sigma_0, Q^{\mathrm{FB}}(\cdot)) = +\infty$.

In Section 3.1 we solve these problems considering ODE system (1),(6) and in Section 3.2 we use ODE-PDE system (1),(10)-(12).

3.1. Optimization problem with ODE system (1),(6)

When using ODE model (1),(6), we assume $\tau_{\mathrm{r}} \gg \tau_{\mathrm{b}}$. We distinguish between the cases in which Q is a constant open-loop control or a feedback control. The case where Q is a time-varying open loop is derived from the case in which Q is a feedback control (as explained in Remark 3.11).

3.1.1. Case 1: Constant open-loop control

Given an initial state $\Sigma_0 = S_{\mathrm{r},0} \in [0, +\infty)$ we look for an optimal constant $Q^{\mathrm{C,opt}} \in \mathcal{Q}^{\mathrm{C}}$ solution of (14). Under assumption (3), if control variable Q is

equivalently replaced by control variable $S_{\mathrm{b}}^{\mathrm{qs}}$ (see Remark 2.2) and if we denote $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}} = \{S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q) \text{ such that } Q \in \mathcal{Q}^{\mathrm{C}}\}$, then problem (14) becomes

$$\begin{cases} \text{Find } S_{\mathrm{b}}^{\mathrm{qs,C,opt}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}} \text{ such that} \\ T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C,opt}}) = \min\limits_{S_{\mathrm{b}}^{\mathrm{qs,C}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C}}} T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}), \end{cases} \tag{16}$$

where $T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}})$ denotes the time required to achieve $S_{\mathrm{r}}(T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}})) = S_{\mathrm{lim}}$ when solving system (1),(6) with the control variable $S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs,C}}$. We now present some theoretical results that are proved in [17], about problem (16).

Lemma 3.7. *If Q is constant (i.e., $S_{\mathrm{b}}^{\mathrm{qs}}$ is constant), one has*

$$T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}) = \frac{1}{\frac{V_{\mathrm{b}}}{V}\mu(S_{\mathrm{b}}^{\mathrm{qs,C}})} \ln\left(\frac{S_{\mathrm{r},0} - S_{\mathrm{b}}^{\mathrm{qs,C}}}{S_{\mathrm{lim}} - S_{\mathrm{b}}^{\mathrm{qs,C}}}\right). \tag{17}$$

Moreover, assuming $S_{\mathrm{r},0} > S_{\mathrm{lim}}$, optimization problem (16) has a unique solution.

Lemma 3.8. ~~*Assuming $S_{\mathrm{r},0} > S_{\mathrm{lim}}$, optimization problem (16) has a unique solution.*~~

We approximate the solution of problem (16) by computing

$$S_{\mathrm{b}}^{\mathrm{qs,C,opt}} = \arg \min_{S_{\mathrm{b}}^{\mathrm{qs,C}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C,N}}} T(S_{\mathrm{r},0}, S_{\mathrm{b}}^{\mathrm{qs,C}}), \tag{18}$$

where $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,C,N}} = \{S_{\mathrm{b},i}^{\mathrm{qs}}\}_{i=1}^{N}$, with $N \in \mathbb{N}$ large enough and $S_{\mathrm{b},i}^{\mathrm{qs}} = \frac{i}{N+1} S_{\mathrm{lim}}$.

3.1.2. Case 2: Feedback control

In this case, we look for an optimal feedback $Q^{\mathrm{FB,opt}} \in \mathcal{Q}^{\mathrm{FB}}$ solution of (15). Under assumption (3), if control variable Q is equivalently replaced by control variable $S_{\mathrm{b}}^{\mathrm{qs}}$ and if we denote $\mathcal{S}_{\mathrm{b}}^{\mathrm{qs,FB}} = \{S_{\mathrm{b}}^{\mathrm{qs}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q) \text{ where } Q \in \mathcal{Q}^{\mathrm{FB}}\}$, then $S_{\mathrm{b}}^{\mathrm{qs,FB,opt}} = S_{\mathrm{b}}^{\mathrm{qs}}(Q^{\mathrm{FB,opt}})$ is called an optimal feedback. As proven in [17], we have the following result.

Lemma 3.9. *An optimal feedback $S_{\mathrm{b}}^{\mathrm{sb,FB,opt}} : [0, +\infty) \to \mathbb{R}$ must fulfill*

$$S_{\mathrm{b}}^{\mathrm{qs,FB,opt}} = \arg \min_{S_{\mathrm{b}}^{\mathrm{qs,FB}} \in \mathcal{S}_{\mathrm{b}}^{\mathrm{qs,FB}}} \frac{V_{\mathrm{b}}}{V} \mu(S_{\mathrm{b}}^{\mathrm{qs,FB}})(S_{\mathrm{b}}^{\mathrm{qs,FB}} - S_{\mathrm{r}}) \tag{19}$$

or, equivalently,

$$\mu'(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}})(S_{\mathrm{r}} - S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}) = \mu(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}). \tag{20}$$

Moreover, $Q^{\mathrm{FB,opt}}(\cdot)$ (see Remark 3.5) is decreasing along any optimal trajectory.

~~If the Monod equation (4) is used we can solve explicitly equation (20) with $S_{\rm b}^{\rm qs,FB,opt}(S_{\rm r}) = \sqrt{K^2 + KS_{\rm r}} - K$.~~

Remark 3.10. *The fact that the open loop realization of the feedback $Q^{\rm FB,opt}$ is decreasing along time can be interpreted physically as follows: as time goes on, the substrate in the water resource is decreasing and the water that enters the bioreactor is less polluted. Therefore, if $Q(\cdot)$ does not decrease, the biomass has not enough time to be in contact with the substrate in order to grow, and eventually becomes extinct.* ~~*Mathematically, when $\frac{Q}{V_{\rm b}} > \mu(S_{\rm r})$, biomass goes asymptotically to the washout equilibrium (see Definition 2.1).*~~

Remark 3.11. *If $Q^{\rm FB,opt}$ is solution of problem (15) when using system (1),(6), given an initial state $\Sigma_0 = S_{\rm r,0} \in [0, +\infty)$, the open-loop representation of $Q^{\rm FB,opt}$ (see Remark 3.5) is solution of problem (14).*

3.2. Optimization problem with ODE-PDE model (1),(10)-(12)

In the case where inhomogeneities are considered, we recall that $S_{\rm out}$ is computed as described in (12). As in Section 3.1, we consider the cases in which Q is chosen as an open-loop control or as a feedback control.

3.2.1. Case 1: Constant open-loop control

Given an initial state $\Sigma_0 \in [0, +\infty) \times (L^\infty(\Omega))^2$ (or $\Sigma_0 \in [0, +\infty)$ for the cases where $\tau_{\rm b} \ll \tau_{\rm r}$, see Remark 3.6), we look for an optimal constant $Q^{\rm C,opt} \in \mathcal{Q}^{\rm C}$ solution of problem (14), that we approximate by taking N equidistant points in the interval $(0, V_{\rm b}\mu(S_{\rm lim}))$ proceeding as in problem (18).

3.2.2. Case 2: Time varying open-loop control

Given an initial state $\Sigma_0 \in [0, +\infty) \times (L^\infty(\Omega))^2$ (or $\Sigma_0 \in [0, +\infty)$ for the cases where $\tau_{\rm b} \ll \tau_{\rm r}$, see Remark 3.6), we look for a time variable function $Q^{\rm OL,opt} \in \mathcal{Q}^{\rm OL}$ close to a solution of (14). With that aim, we consider a family of time varying functions with 5 optimization parameters, denoted by Q_0, Q_1, Q_2, Q_3 and Q_4. Those optimization parameters correspond to the value of the flow rate $Q^{\rm OL}(\cdot)$ at five different given fixed times t_0, t_1, t_2, t_3 and t_4, starting from time $t_0 = 0$, so that function $Q^{\rm OL}$ is given by $Q^{\rm OL}(t_i) = Q_i$ $(i = 0, \ldots, 4)$, $Q^{\rm OL}(t)$ is calculated with the *monotone piecewise cubic hermite interpolation* method, with null derivatives at t_0 and t_4 (see for instance [37]) for $t \in (t_i, t_{i+1})$ $(i = 0, \ldots, 3)$, and $Q^{\rm OL}(t) = Q_4$ for $t \geq t_4$.

$$Q^{\rm OL}(t) = \begin{cases} Q_0 & \text{if} \quad t = 0, \\ Q_1 & \text{if} \quad t = t_1, \\ Q_2 & \text{if} \quad t = t_2, \\ Q_3 & \text{if} \quad t = t_3, \\ Q_4 & \text{if} \quad t \geq t_4 \end{cases}$$

Following Remark 3.10, we only consider decreasing time functions $Q(\cdot)$. Thus, we compute the optimization parameters Q_0, Q_1, Q_2, Q_3 and Q_4 with the

following constraints

$$Q_0 > Q_1 > Q_2 > Q_3 > Q_4.$$

To that end, we consider the optimization parameter $Q_0 \in [0, V_b\mu(S_{r,0}))$ and we define new optimization parameters α_1, α_2, α_3 and α_4 in $[0, 1]$ such that the interpolation data are given by

$$Q_1 = \alpha_1 Q_0, \qquad Q_2 = \alpha_2 Q_1, \qquad Q_3 = \alpha_3 Q_2, \qquad Q_4 = \alpha_4 Q_3.$$

Therefore, we approximate $Q^{\mathrm{OL,opt}}(\cdot)$ by a function defined by interpolation, as explained above, and where the corresponding vector $\gamma^{\mathrm{opt}} = (Q_0^{\mathrm{opt}}, \alpha_1^{\mathrm{opt}}, \alpha_2^{\mathrm{opt}}, \alpha_3^{\mathrm{opt}}, \alpha_4^{\mathrm{opt}})$ is solution of

$$\begin{cases} \text{Find } \gamma^{\mathrm{opt}} \in (0, V_b\mu(S_{r,0})) \times (0,1)^4 \text{ such that} \\ T(\Sigma_0, Q^{\mathrm{OL,opt}}(\cdot)) = \min\limits_{\gamma \in (0, V_b\mu(S_{r,0})) \times (0,1)^4} T(\Sigma_0, Q^{\mathrm{OL}}(\cdot)), \end{cases} \tag{21}$$

where $T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))$ denotes the time required to achieve $S_r(T(\Sigma_0, Q^{\mathrm{OL}}(\cdot))) = S_{\lim}$ when solving (with any suitable solver; see e.g. Section 4.1) system (1) coupled with (10)-(12) with the flow rate $Q = Q^{\mathrm{OL}}(\cdot)$. We solve problem (21) with the Hybrid Genetic Algorithm (HGA), and its parameters, presented in [32]. The HGA is a global optimization algorithm based on a combination between a Genetic Algorithm (which, without requiring the computation of the gradient of the cost function, performs a first coarse global search of the solution) and a Steepest Descent method (which performs a refined local search of the solution). The suitability of this method to solve computationally expensive optimization problems has been shown in [38].

Remark 3.12. ~~*We have used other approaches for computing time varying open-loop solutions of problem (14), for instance $Q(t) = \frac{1}{(At+B)^p}$, where A, B, p are in a suitable search space. Nevertheless, in the following we do not present the optimization results obtained with this approach since they are not better than those obtained with the approach explained above.*~~

3.2.3. Case 3: Feedback Approximation

In this case, we look for an optimal feedback $Q^{\mathrm{FB,opt}} \in \mathcal{Q}^{\mathrm{FB}}$ solution of problem (15). To this end, proceeding similarly as done in Lemma 3.9 for perfectly mixed bioreactors, we perform a suboptimal strategy as a greedy policy that consists in choosing a control maximizing the instantaneous decrease of the contaminant concentration in the resource.
For cases where $\tau_b \ll \tau_r$, we assume that the feedback only depends on S_r, i.e., $\Sigma = S_r$ (see Remark 3.6) and we approximate the feedback function that we are looking for by solving the following optimization problem: Given an arbitrary resource substrate concentration $S \in [0, +\infty)$ and a small time interval $\Delta t > 0$ (chosen of the order of the water resource time scale τ_r in order to assure that the bioreactor is in quasi-steady state during the time interval Δt)

$$\begin{cases} \text{Find } Q^{\mathrm{FB,opt}}(S) \in [0, V_b\mu(S)) \text{ such that} \\ \\ S_r(S, Q^{\mathrm{FB,opt}}; \Delta t) = \min_{Q^{\mathrm{FB}} \in [0, V_b\mu(S))} S_r(S, Q^{\mathrm{FB}}; \Delta t), \end{cases} \tag{22}$$

where $S_{\mathrm{r}}(S, Q^{\mathrm{FB}}; \Delta t)$ is the solution (computed with any suitable solver; see e.g Section 4.1) of system (1) coupled with (10)-(12) at time Δt, with $S = S_0$ and $Q = Q^{\mathrm{FB}}(S)$. Since $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ the bioreactor is in quasi-steady state and the choice of the concentration values $S_{\mathrm{b},0}$ and $B_{\mathrm{b},0}$ does not have influence on the solution of problem (22). Particularly, we take $S_{\mathrm{b},0} = B_{\mathrm{b},0} = S$. We estimate the solution of problem (22) by taking N equidistant points in the interval $(0, V_{\mathrm{b}}\mu(S))$ and proceeding as in problem (18). Then, in order to obtain a function of the form

$$\begin{array}{rccl} Q^{\mathrm{FB,opt}}: & [S_{\mathrm{lim}}, S_{\mathrm{r},0}] & \longrightarrow & [0, V_{\mathrm{b}}\mu(S_{\mathrm{r},0})) \\ & S & \to & Q^{\mathrm{FB,opt}}(S), \end{array} \tag{23}$$

we solve problem (22) for a range of concentration values $S \in \mathcal{S} = \{S_i\}_{i=1}^{I+1}$, where $I \in \mathbb{N}$ is large enough and $S_i = S_{\mathrm{r},0} - \frac{i-1}{I}(S_{\mathrm{r},0} - S_{\mathrm{lim}})$. Finally, $Q^{\mathrm{FB,opt}}(S)$ is calculated with the *monotone piecewise cubic hermite interpolation* with null derivatives at S_{lim} and $S_{\mathrm{r},0}$ (see [37]) for $S \notin \mathcal{S}$.

For cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ is not satisfied, we approximate the feedback function that we are looking for by solving the following optimization problem: Given arbitrary concentration values $(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \in [0, +\infty) \times (L^\infty(\Omega))^2$ and a small time interval $\Delta t > 0$

$$\begin{cases} \text{Find } Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \in [0, V_{\mathrm{b}}\mu(S)) \text{ such that} \\ \\ S_{\mathrm{r}}(\Sigma, Q^{\mathrm{FB,opt}}; \Delta t) = \min_{Q^{\mathrm{FB}} \in [0, V_{\mathrm{b}}\mu(S))} S_{\mathrm{r}}(S, Q^{\mathrm{FB}}; \Delta t), \end{cases} \tag{24}$$

where $S_{\mathrm{r}}(S, Q^{\mathrm{FB}}; \Delta t)$ is the solution (obtained with a suitable numerical solver; see e.g. Section 4.1) of system (1) coupled with (10)-(12) at time Δt, with $\Sigma_0 = (S, s_{\mathrm{b}}, b_{\mathrm{b}})$ and $Q = Q^{\mathrm{FB}}(S, s_{\mathrm{b}}, b_{\mathrm{b}})$. We estimate the solution of problem (24) by taking N equidistant points in the interval $(0, V_{\mathrm{b}}\mu(S))$ and proceeding as in problem (18).
Then, in order to obtain a function of the form

$$\begin{array}{rccl} Q^{\mathrm{FB,opt}}: & [S_{\mathrm{lim}}, S_{\mathrm{r},0}] \times (L^\infty(\Omega))^2 & \longrightarrow & [0, V_{\mathrm{b}}\mu(S_{\mathrm{r},0})) \\ & (S, s_{\mathrm{b}}, b_{\mathrm{b}}) & \to & Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}}), \end{array} \tag{25}$$

we solve problem (24) for a range of concentration values $(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ in the set $\mathcal{M} = \{(S, s_{\mathrm{b}}, b_{\mathrm{b}}) : \exists i \in \{1, \ldots, I+1\}$ such that $S = S_i \in \mathcal{S}$, $s_{\mathrm{b}} \in \mathcal{S}_{\mathrm{b},i}$ and $b_{\mathrm{b}} \in \mathcal{B}_{\mathrm{b},i}\}$ where $S_i = S_{\mathrm{r},0} - \frac{i-1}{I}(S_{\mathrm{r},0} - S_{\mathrm{lim}})$, $\mathcal{S}_{\mathrm{b},i} = \mathcal{B}_{\mathrm{b},i} = \{S_{i,j}\}_{j \in J}$ with $J \subset \mathbb{N}$ and $S_{i,j} = \frac{S_i}{j}$. If $(S, s_{\mathrm{b}}, b_{\mathrm{b}}) \notin \mathcal{M}$, we compute the mean value of the concentrations s_{b} and b_{b} in the bioreactor (which we denote by $\overline{s}_{\mathrm{b}}$ and $\overline{b}_{\mathrm{b}}$) by

$$\overline{s}_{\mathrm{b}} = \frac{2\displaystyle\int_0^L \int_0^H r s_{\mathrm{b}}(r, z)\, \mathrm{d}z\mathrm{d}r}{L^2 H}, \quad \overline{b}_{\mathrm{b}} = \frac{2\displaystyle\int_0^L \int_0^H r b_{\mathrm{b}}(r, z)\, \mathrm{d}z\mathrm{d}r}{L^2 H},$$

and $Q^{\mathrm{FB,opt}}(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ is approximated by $Q^{\mathrm{FB,opt}}(S, \overline{s}_{\mathrm{b}}, \overline{b}_{\mathrm{b}})$, which is given by *spatial interpolation*. More specifically, $Q^{\mathrm{FB,opt}}(S, \overline{s}_{\mathrm{b}}, \overline{b}_{\mathrm{b}})$ is calculated with a suitable *trilinear* or *neighbor interpolation* method depending if $(S, s_{\mathrm{b}}, b_{\mathrm{b}})$ is or not inside the convex hull of $\mathcal{M}$.

Remark 3.13. ~~*Set $\mathcal{M}$ has been chosen following the stability analysis of the ODE system (5), presented in Section 2.2.1, which shows that the value of concentration of both substrate and biomass at their equilibria state is below the substrate concentration in the resource. Nevertheless, in order to obtain a function of the form (25), the same methodology can be applied with more general sets $\mathcal{M}$.*~~

Remark 3.14. *Solution of problems (22) and (24) are approximations of the solution of problem (15) which, as shown in Section 4.3, provide satisfactory results.*

4. Numerical Experiments

In this section, we first introduce the numerical solvers used for computing the solutions of systems (1),(6) and (1),(10)-(12). Then, in Sections 4.2 and 4.3 we present the numerical results obtained when looking for constant and feedback controls, respectively. Notice that in order to shorten the presentation of this work, the results obtained when looking for time varying open-loop controls has been included in Section 4.3.

4.1. Numerical solvers used for systems (1),(6) and (1),(10)-(12)

The solution of system (1),(6) was computed numerically by using a fourth-order Runge-Kutta method and the solution of system (1),(10)-(12) was computed numerically by coupling a fourth-order Runge-Kutta method with a Finite Element Method (see [39]). The computational experiments were carried out with a 2.8Ghz Intel i7-930 64bits computer with 12Gb of RAM. We used a triangular mesh with around 600 elements. A numerical simulation of system (1),(10)-(12) with time step $\Delta t = 100$s and final time 10^5s, computed using MATLAB (`mathworks.com`) and COMSOL Multyphisics 5.0 (`www.comsol.com`), takes approximately 12 seconds.

Model parameters were taken following [17, 19]: $\mu(\cdot)$ was the Monod Function (see (4)) with $\mu_{\max} = 1$ (s^{-1}) and $K = 1$ ($\mathrm{mol/m}^3$). For the bioreactor and water resource volumes we took $V_{\mathrm{b}} = 1$ (m^3) and $V = 1000$ (m^3), respectively. In order to obtain a cylinder of volume $V_{\mathrm{b}} = 1$ (m^3), we used a 2D bioreactor domain with $H = L = 0.68$ (m). We considered a case for which the time scale of the bioreactor was comparable to the time scale of the water resource by using diffusion coefficients $D_{\mathrm{S}} = D_{\mathrm{B}} = 0.01$ (m^2/s). We also consider a case where the time scale for the bioreactor was much smaller than the time scale of the water resource by using diffusion coefficients $D_{\mathrm{S}} = D_{\mathrm{B}} = 100$ (m^2/s). When computing a constant open loop control (see Section 3.2.1), $N = 100$ was chosen to solve

problem (18). When computing a time-varying open loop (see Section 3.2.2), the interpolation times were $t_0 = 0$ (s), $t_1 = 20000$(s), $t_2 = 40000$(s), $t_3 = 60000$(s) and $t_4 = 80000$(s). Those values where taken equidistant and having estimated experimentally that the time needed to achieve the prescribed value in the resource is around 10^5s. Finally, when computing a feedback (see Section 3.2.3), problems (22) and (24) were solved by using the MATLAB functions `interp1` and `interp3` (see `https://www.mathworks.com/moler/interp.pdf`), respectively, with $\Delta t = 100$ s.

Remark 4.1. *The model parameters considered here were chosen as in [17] in order to obtain a straightforward comparison between the methodologies proposed in this article and the ones introduced here. Of course, they could be replaced by other values found in the literature.*

4.2. Constant Open-Loop Control

In this Section, we solve numerically the optimization problem (14) when the volumetric flow rate Q is considered a constant. More specifically, Section 4.2.1 shows the numerical results for the ODE system (1),(6), obtained by solving problem (18), and Section 4.2.2 shows the numerical results for the ODE-PDE system (1),(10)-(12), obtained as explained in Section 3.2.1. Then, in Section 4.2.3 we make a comparison of the results obtained in Sections 4.2.1 and 4.2.2 in terms of the optimal constant open-loop controls and the time needed to achieve the prescribed value of substrate concentration in the water resource, S_{lim}. We also compare systems (1),(6) and (1),(10)-(12) in terms of the minimum substrate concentration achieved in the water resource if the constant flow rate obtained for system (1),(6) is used in system (1),(10)-(12). Simulations were done with initial substrate concentration in the resource $S_{\text{r},0}$~~= 5 and 10~~ (mol/m^3) and with $S_{\text{lim}} = 0.1$ (mol/m^3). These simulations were also performed for $S_{\text{r},0} = 5$ (mol/m^3) and similar conclusions were obtained.

4.2.1. ODE system (1),(6)

In this Section we solve the optimization problem (18) using system (1),(6) with $N = 200$. The optimal constant open-loop is $Q_{\text{ODE}}^{\text{C,opt}} = 0.0790$ (m^3/s) and the corresponding decontamination time is $T(S_{\text{r},0}, Q_{\text{ODE}}^{\text{C,opt}}) = 81830$ (s). ~~Table 1 shows the results.~~

~~$S_{\text{r},0}$ (mol/m^3)~~	~~$Q_{\text{ODE}}^{\text{C,opt}}$ (m^3/s)~~	~~$T(S_{\text{r},0}, Q_{\text{ODE}}^{\text{C,opt}})(s)$~~
~~5~~	~~0.0776~~	~~74090~~
~~10~~	~~0.0790~~	~~81830~~

Table 1: ~~ODE model: Value of the optimal constant open-loop $Q_{\text{ODE}}^{\text{C,opt}}$ and the corresponding decontamination time for two different initial values $S_{\text{r},0}$.~~

4.2.2. ODE-PDE model (1),(10)-(12)

In this Section we solve the optimization problem (14) using the model given by system (1),(10)-(12). We denote $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ the optimal constant flow rates when considering the homogeneous and the nonhomogeneous flow velocity fields, respectively. Equivalently, we denote $S_{\mathrm{r,ach}}^{\mathrm{H}}$ and $S_{\mathrm{r,ach}}^{\mathrm{NH}}$ the minimum substrates concentrations achieved in the water resource if $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in system (1),(10)-(12). For these concentration values, the flow rate $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is high enough to drive system (1),(10)-(12) to washout (see Definition 2.1), i.e., the biomass become extinct and no more reaction is produced.

We distinguish between the cases where the time scale of the bioreactor is much smaller than the time scale of the water resource (i.e., $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$) and the case where that condition is not satisfied.

- **Case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$:**
  Table 2 shows optimal constant open loops and the corresponding decontamination times ~~and Table 3 shows the substrate concentrations achieved in the resource.~~ The substrate concentrations achieved in the resource are $S_{\mathrm{r,ach}}^{\mathrm{H}} = 0.08569$ (mol/m^3) and $S_{\mathrm{r,ach}}^{\mathrm{NH}} = 0.1177$ (mol/m^3).

$S_{\mathrm{r},0}$ (mol/m^3)	$Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{H}}^{\mathrm{C,opt}})$ (s)	$Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{NH}}^{\mathrm{C,opt}})$ (s)
~~5~~	~~0.0758~~	~~72750~~	~~0.0581~~	~~98490~~
10	0.0778	81840	0.0594	110420

Table 2: ODE-PDE model: case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$. Values of the optimal constant open-loops $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the corresponding decontamination times for ~~two initial values~~ $S_{\mathrm{r},0}$~~=~~ 10 (mol/m^3).

~~$S_{\mathrm{r},0}$ (mol/m^3)~~	~~$S_{\mathrm{r,ach}}^{\mathrm{H}}$ (mol/m^3)~~	~~$S_{\mathrm{r,ach}}^{\mathrm{NH}}$ (mol/m^3)~~
~~5~~	~~0.08404~~	~~0.1153~~
~~10~~	~~0.08569~~	~~0.1177~~

Table 3: ~~ODE-PDE model: case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$. Substrate concentrations achieved if the constant flow rate $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in system (1),(10)-(12) for two initial values $S_{\mathrm{r},0}$~~.

- **Case $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$:**
  In this case, the optimal constant open loop also depends on the initial state at the bioreactor. Since we aim to compare the optimal constant open-loop controls obtained for the ODE system (1),(6) and the ODE-PDE system (1),(10)-(12), we estimate a function of the form $S_{\mathrm{r},0} \to Q_{\mathrm{H}}^{\mathrm{C,opt}}(S_{\mathrm{r},0})$ by solving problem (14) for a range of initial states in the set $\mathcal{M}$ defined to solve problem (24) with $I = 1$ and $J = \{1, 2, 4, 10\}$. Then,

$Q_{\mathrm{H}}^{\mathrm{C,opt}}$ is approximated by computing the mean value of the set of optimal constant open-loop controls obtained for the different initial states. This procedure is also used to obtain the optimal constant $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the substrate concentrations $S_{\mathrm{r,ach}}^{\mathrm{H}}$ and $S_{\mathrm{r,ach}}^{\mathrm{NH}}$.
Table 4 shows the optimal constant flow rates and the corresponding decontamination times ~~and Table 5 shows the substrate concentrations achieved in the resource.~~ The substrate concentrations achieved in the resource are $S_{\mathrm{r,ach}}^{\mathrm{H}} = 0.1524$ (mol/m^3) and $S_{\mathrm{r,ach}}^{\mathrm{NH}} = 0.1776$ (mol/m^3).

$S_{\mathrm{r},0}$ (mol/m^3)	$Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{H}}^{\mathrm{C,opt}})$ (s)	$Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ (m^3/s)	$T(S_{\mathrm{r},0}, Q_{\mathrm{NH}}^{\mathrm{C,opt}})$ (s)
~~5~~	~~0.0540~~	~~89260~~	~~0.0435~~	~~113390~~
10	0.0547	102190	0.0442	129160

Table 4: ODE-PDE model: case $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$. Values of the optimal constant open-loops $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$ and the corresponding decontamination times for ~~two different initial values~~ $S_{\mathrm{r},0}$= 10 (mol/m^3).

~~$S_{\mathrm{r},0}$ (mol/m^3)~~	~~$S_{\mathrm{r,ach}}^{\mathrm{H}}$ (mol/m^3)~~	~~$S_{\mathrm{r,ach}}^{\mathrm{NH}}$ (mol/m^3)~~
~~5~~	~~0.14811~~	~~0.1738~~
~~10~~	~~0.1524~~	~~0.1776~~

Table 5: ~~ODE-PDE model: case $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$. Substrate concentration achieved if the constant $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in system (1),(10)-(12)for two different initial values $S_{\mathrm{r},0}$.~~

4.2.3. Discussion

An interesting study is to check if the optimization results obtained in Sections 4.2.1 and 4.2.2 are similar. We make the comparison for both flow velocity fields, described in Section 2.2.2.

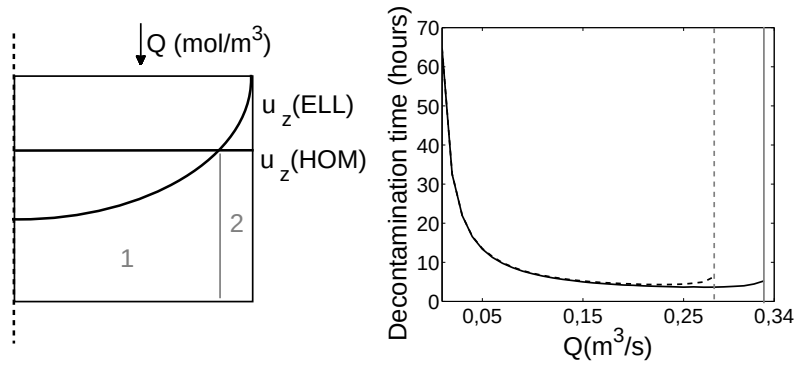
- **Homogenous flow velocity field**: We can observe from results in Section 4.2.1 and Table 2 that the volumetric flow rates $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (obtained with the ODE-PDE system (1),(10)-(12) when $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$) are significantly close and the decontamination times are comparable (the difference is below 1% for both values of $S_{\mathrm{r},0}$). Nevertheless, from results in Section 4.2.1 and Table 4 one notice that the flow rate $Q_{\mathrm{H}}^{\mathrm{C,opt}}$ (obtained with the ODE-PDE system (1),(10)-(12) when $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$) is around 70% of the value of $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$. Furthermore, from the values $S_{\mathrm{r,ach}}^{\mathrm{H}}$ we conclude that if the constant $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is applied in system (1),(10)-(12) in the case where $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$, the bioreactor is driven to washout (see Definition 2.1) before the decontamination target is achieved. These results seem to indicate that when high diffusions are considered, the optimal constant controls obtained with the ODE model are similar to those obtained with the ODE-PDE model, whereas for low diffusion coefficients the ODE-PDE

model exhibits better results, in the sense that it provides smaller volumetric flow rates which favor that the biomass does not become extinct in the bioreactor before the target is achieved (see Remark 3.3).

- **Nonhomogeneous flow velocity field**: We can observe from results in Section 4.2.1 and Tables 2 and 4 that the volumetric flow rates $Q_{\mathrm{NH}}^{\mathrm{C,opt}}$, obtained with the ODE-PDE system (1),(10)-(12) in the cases where $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$ and $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$, are around 75% and 60% of the value of the flow rate $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$, respectively. Furthermore, from the values $S_{\mathrm{r,ach}}^{\mathrm{NH}}$ we conclude that if the constant $Q_{\mathrm{ODE}}^{\mathrm{C,opt}}$ is used in the ODE-PDE system (1),(10)-(12), the bioreactor is driven to washout (see Definition 2.1) before the decontamination target is achieved. These results seem to indicate that when the nonhomogeneous flow velocity field is considered, model (1),(10)-(12) exhibits better results, in the sense that it provides smaller volumetric flow rates which favor that the biomass does not become extinct in the bioreactor before the target is achieved (see Remark 3.3). ~~The influence of the nonhomogeneous flow velocity field in the washout phenomena is explained in Remark 4.2.~~

Remark 4.2. ~~*We recall from Section 2.2 that the washout phenomena (see Definition 2.1) is produced when $Q(t) \geq V_{\mathrm{b}}\mu(S_{\mathrm{r}}(t))$. It is reasonable to assume that for high diffusion coefficients D_{S} and D_{B}, the substrate and biomass concentrations become homogeneous in the bioreactor so that the ODE-PDE model (1),(10)-(11) approaches the ODE model (9), and consequently, the washout is also produced when $Q(t) \geq V_{\mathrm{b}}\mu(S_{\mathrm{r}}(t))$. Nevertheless, this analogy only takes place when using the homogeneous flow velocity field in system (1),(10)-(12). As detailed in Section 2.2.2, the nonhomogeneous flow velocity field is taken as $u_z(r,t) = -\frac{3Q(t)\sqrt{L^2-r^2}}{3L^3}$, so it attains its maximum depth at $r = 0$. This maximum depth is $\frac{3}{2}$ the maximum depth if the homogeneous profile is taken, so we can conclude that when using the nonhomogeneous flow velocity field, washout occurs for $Q(t) \geq Q_{\max}(t)$, where $Q_{\max}(t)$ is some value in the interval $[\frac{2}{3}V_{\mathrm{b}}\mu(S_{\mathrm{r}}(t)), V_{\mathrm{b}}\mu(S_{\mathrm{r}}(t))]$. In order to find a physical explanation, we observe Figure 4-(a), pointing out that if the nonhomogeneous flow velocity field is used, the liquid located in region 1 is ejected from the bioreactor faster than if we use the homogeneous flow velocity field. Thus, the substrate is in contact with the biomass less time and consequently the water remains polluted in this region when going out from the reactor. Furthermore, due to diffusion, the particles situated in the regions 1 and 2 are mixed and the resulting contamination value is higher than the required threshold. Figure 4-(b) shows the difference in terms of decontamination time between using the homogeneous and the nonhomogeneous flow velocity fields when Q (m^3/s) is considered constant ($Q \in \mathcal{Q}^{\mathrm{C}}$). Particularly, taking $S_{\mathrm{r},0} = 5$ (mol/m^3) and the objective value $S_{\mathrm{lim}} = 0.5$ (mol/m^3), one obtains that in order to avoid washout Q should be in the interval $[0, 0.33)$. We observe that the washout phenomena starts at the value $Q \approx 0.33$ in the case of considering the homogeneous flow velocity field, but starts earlier if we use the*~~

~~*nonhomogeneous flow velocity field.*~~



(a) ~~Typical homogeneous and nonhomogeneous flow velocity fields~~

(b) ~~Decontamination times obtained by using the homogeneous flow velocity field (depicted by a solid line) or the ellipsoid flow velocity field (depicted by a dashed line). Notice that the vertical lines are allocated at the value of Q for which washout starts.~~

Figure 4: ~~Scheme of the washout phenomena when using the homogeneous and the nonhomogeneous flow velocity fields.~~

4.3. Feedback

In this Section, we look for an optimal feedback, denoted by $Q^{\mathrm{FB,opt}}$ solution of problem (15). More specifically, Section 4.3.1 shows the results for the ODE system (1),(6), obtained using Lemma 3.9 and Section 4.3.2 shows the feedback approximations for the ODE-PDE system (1),(10)-(12), obtained when solving the suboptimal problems (22) and (24). Section 4.3.2 also shows the feedback synthesis (see definition below) of the optimal time varying open-loops, obtained when solving (21). Then, in Section 4.3.3 we make a comparison of the results presented in Sections 4.3.1 and 4.3.2 in terms of the feedback control. Furthermore, we compare models (1),(6) and (1),(10)-(12) in terms of the minimum substrate concentration achieved in the water resource if the optimal feedback obtained for system (1),(6) is used in system (1),(10)-(12).

4.3.1. ODE model (1),(6)

As detailed in Section 3.1.2 if the Monod equation (4) is taken, the optimal feedback, denoted by $Q^{\mathrm{FB,opt}}_{\mathrm{ODE}}$, fulfills

$$Q^{\mathrm{FB,opt}}_{\mathrm{ODE}} = V_{\mathrm{b}}\mu(S_{\mathrm{b}}^{\mathrm{qs,FB,opt}}) = V_{\mathrm{b}}\mu(\sqrt{K^2 + K \cdot S_{\mathrm{r}}} - K).$$

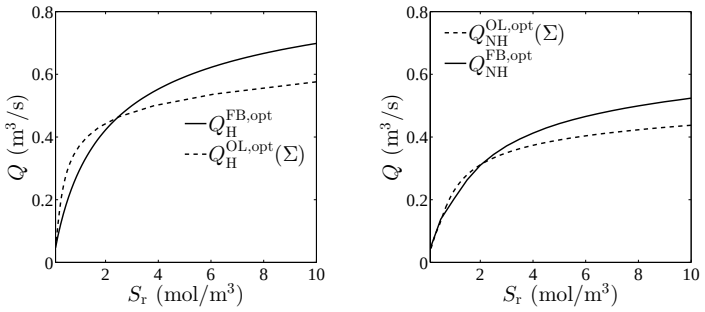
4.3.2. ODE-PDE model (1),(10)-(12)

As a first approach, we solve problem (15) by solving optimization problems (22) and (24) (considering a feedback approximation, as described in Section

3.2.3), for both homogeneous and nonhomogeneous flow velocity fields, denoting the solution by $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{FB,opt}}$, respectively.
In order to compare with time varying open-loop controls (see Section 3.2.2), as a second approach we solve problem (15) by solving the optimization problem (21) and then taking the feedback synthesis of the time varying open-loop, i.e., for any time t with corresponding values $Q(t)$ and $\Sigma(t)$, we can reconstruct the map $\Sigma(t) \to Q(t)$, that can be seen as a state-dependent control function, which in the following we denote by $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$ and $Q_{\mathrm{NH}}^{\mathrm{OL,opt}}(\Sigma)$, for the homogeneous and the nonhomogeneous flow velocity fields, respectively. Equivalently, we denote $S_{\mathrm{r,ach}}^{\mathrm{H}}$ and $S_{\mathrm{r,ach}}^{\mathrm{NH}}$ the minimum substrate concentrations achieved in the water resource if $Q_{\mathrm{ODE}}^{\mathrm{FB,opt}}$ is used in system (1),(10)-(12). For these concentration value, the flow rate $Q_{\mathrm{FB,opt}}^{\mathrm{ODE}}$ is high enough to drive system (1),(10)-(12) to washout (see Definition 2.1), i.e., the biomass become extinct and no more reaction is produced.

Simulations have been conducted for substrate concentration $S_{\mathrm{r},0} = 10$ (mol/m^3) $S_{\mathrm{lim}} = 0.1$ (mol/m^3).

- **Case** $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$
  Figure 5 shows the similarities between the feedbacks obtained with the two approaches described above. More precisely, Figure 5-(a) shows the feedbacks $Q_{\mathrm{H}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{H}}^{\mathrm{OL,opt}}(\Sigma)$ and Figure 5-(b) shows the feedbacks $Q_{\mathrm{NH}}^{\mathrm{FB,opt}}$ and $Q_{\mathrm{NH}}^{\mathrm{OL,opt}}(\Sigma)$, while the corresponding decontamination times are shown in Table 6. Note that, for the sake of comparison, Table 6 also includes the decontamination times $T(S_{\mathrm{r},0}, Q_{\mathrm{ODE}}^{\mathrm{C,opt}})$, obtained in Section 4.2.1.



(a) Homogeneous flow velocity field (b) Nonhomogeneous flow velocity field

Figure 5: ODE-PDE model: case $\tau_{\mathrm{b}} \ll \tau_{\mathrm{r}}$. Comparison between the feedback approximations $Q^{\mathrm{FB,opt}}$ (depicted with solid lines) and $Q^{\mathrm{OL,opt}}$ (depicted with dashed lines).

- **Case** $\tau_{\mathrm{b}} \approx \tau_{\mathrm{r}}$:
  In this case, time varying open loops and feedbacks depend on the bioreactor state. Since we aim to compare the optimal feedback obtained for

$T(S_{r,0}, Q_H^{FB,opt})$ (s)	$T(S_{r,0}, Q_H^{OL,opt})$ (s)	$T(S_{r,0}, Q_H^{C,opt})$ (s)
49870	48040	81840
$T(S_{r,0}, Q_{NH}^{FB,opt})$ (s)	$T(S_{r,0}, Q_{NH}^{OL,opt})$ (s)	$T(S_{r,0}, Q_{NH}^{C,opt})$ (s)
64770	63990	110420

Table 6: ODE-PDE model: case $\tau_b \ll \tau_r$. Decontamination times obtained with system (1),(10)-(12), $S_{r,0} = 10$ (mol/m^3) and controls $Q^{FB,opt}$, $Q^{OL,opt}$ and $Q^{C,opt}$.

ODE model (1),(6) with the two feedback schemes obtained for ODE-PDE model (1),(10)-(12), we approximate functions of the form $S_r \to Q_H^{FB,opt}(S_r)$ and $S_{r,0} \to Q_H^{OL,opt}(S_{r,0};\cdot)$. In order to compute $Q_H^{FB,opt}(S_r)$ (or $Q_{NH}^{FB,opt}(S_r)$) we solve problem (24) for (S, s_b, b_b) in the set $\mathcal{M}$, defined to solve problem (22), with $I = 20$ and $J = \{1, 2, 4, 10\}$. Thus, for each $S \in \mathcal{S}$, $Q^{FB,opt}(S)$ is approximated by computing the mean value of the set of optimal feedbacks $Q^{FB,opt}(S, s_b, b_b)$ with $(S, s_b, b_b) \in \mathcal{M}$. Similarly, in order to compute $Q_H^{OL,opt}(S_{r,0};\cdot)$ we solve problem (21), taking $\Sigma_0 \in \mathcal{M}$ with $I = 1$ and $J = \{1, 2, 4, 10\}$. Then, each component of vector γ^{opt} is approximated by computing the mean value of the set of its optimal values obtained for the different initial states. This procedure is also used to obtain the average optimal time varying open loop $Q_{NH}^{C,opt}(S_{r,0};\cdot)$ and substrate concentrations $S_{r,ach}^{H}$ and $S_{r,ach}^{NH}$.

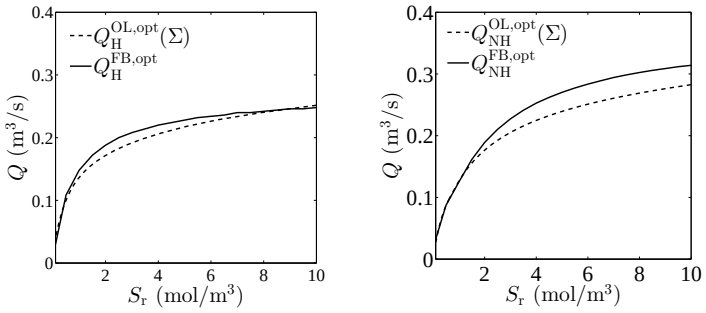
Figure 6 shows the similarities between the feedbacks obtained with the two approaches described above. More precisely, Figure 6-(a) shows the feedbacks $Q_H^{FB,opt}$ and $Q_H^{OL,opt}(\Sigma)$, obtained when considering the homogeneous flow velocity field. Figure 6-(b) shows the feedbacks $Q_{NH}^{FB,opt}$ and $Q_{NH}^{OL,opt}(\Sigma)$, obtained when considering the nonhomogeneous flow velocity field. The corresponding decontamination times are shown in Table 8. Note that, for the sake of comparison, Table 8 also includes the decontamination times $T(S_{r,0}, Q_{ODE}^{C,opt})$, obtained in Section 4.2.1. The substrate concentrations achieved in the resource are $S_{r,ach}^{H} = 9.9888$ (mol/m^3) and $S_{r,ach}^{NH} = 9.9836$ (mol/m^3). ~~Table 7 shows the substrate concentrations achieved in the resource.~~

~~$S_{r,0}$ (mol/m^3)~~	~~$S_{r,ach}^{H}$ (mol/m^3)~~	~~$S_{r,ach}^{NH}$ (mol/m^3)~~
~~10~~	~~9.9888~~	~~9.9836~~

Table 7: ~~ODE-PDE model: Case $\tau_b \approx \tau_r$. Substrate concentration achieved if the feedback $Q_{ODE}^{FB,opt}$ is used in System (1),(10)-(12).~~

4.3.3. Discussion

An interesting study is to check if both approaches, described in Sections 3.2.2 and 3.2.3, present similar numerical results. From Figure 5 and Figure 6 one can observe significant similarities between the two volumetric flow rates



(a) Homogeneous flow velocity field (b) Nonhomogeneous flow velocity field

Figure 6: ODE-PDE model: Case $\tau_{\rm b} \approx \tau_{\rm r}$. Comparison between the feedback approximations $Q^{\rm FB,opt}$ (depicted with solid lines) and $Q^{\rm OL,opt}(\Sigma)$ (depicted with dashed lines).

$T(S_{\rm r,0}, Q_{\rm H}^{\rm FB,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm H}^{\rm OL,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm H}^{\rm C,opt})$ (s)
58900	57610	102190
$T(S_{\rm r,0}, Q_{\rm NH}^{\rm FB,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm NH}^{\rm OL,opt})$ (s)	$T(S_{\rm r,0}, Q_{\rm NH}^{\rm C,opt})$ (s)
74050	74180	129160

Table 8: ODE-PDE model: case $\tau_{\rm b} \ll \tau_{\rm r}$. Decontamination times obtained with system (1),(10)-(12), $S_{\rm r,0} = 10$ (mol/m^3) and controls $Q^{\rm FB,opt}$, $Q^{\rm OL,opt}$ and $Q^{\rm C,opt}$.

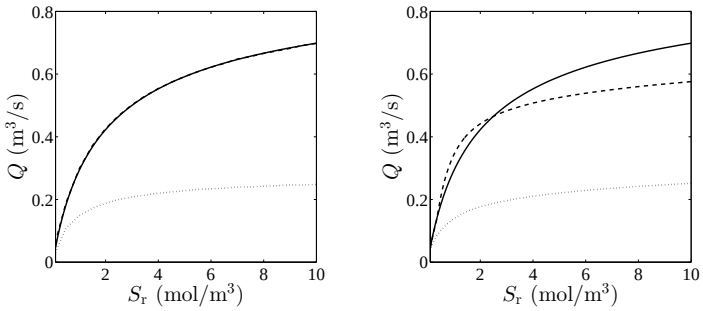
$Q^{\rm FB,opt}$ and $Q^{\rm OL,opt}(\Sigma)$, being the first one a bit faster than the second one in most of the cases. This result is not surprising, since the open-loop approach takes into account the concentrations only at initial time, while the feedback strategy is intrinsically more robust.

Another interesting study is to check if the optimization results obtained in Sections 4.3.1 and 4.3.2 are similar. We make the comparison for both flow velocity profiles, described in Section 2.2.2.

- **Homogenous flow velocity field**: In order to analyze the similarities between the obtained optimal controls $Q_{\rm ODE}^{\rm FB,opt}$, $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm H}^{\rm OL,opt}(\Sigma)$, we plot them in Figure 7. It is easy to observe that the volumetric flow rates $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm H}^{\rm OL,opt}(\Sigma)$ (obtained with the ODE-PDE system (1),(10)-(12) in the case where $\tau_{\rm b} \ll \tau_{\rm r}$) are significantly close to the flow rate $Q_{\rm ODE}^{\rm FB,opt}$ (in fact, $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm ODE}^{\rm FB,opt}$ seem indistinguishable in Figure 7-(a)). Nevertheless, the flow rates $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm H}^{\rm OL,opt}(\Sigma)$ (obtained with the ODE-PDE system (1),(10)-(12) when $\tau_{\rm b} \approx \tau_{\rm r}$) are much slower than $Q_{\rm ODE}^{\rm FB,opt}$. For instance, for $S_{\rm r} = 10$ (mol/m^3) the values of $Q_{\rm H}^{\rm FB,opt}$ and $Q_{\rm H}^{\rm OL,opt}(\Sigma)$ are around 35% the value of $Q_{\rm ODE}^{\rm FB,opt}$. Furthermore, from the value $S_{\rm r,ach}^{\rm H}$, we conclude that if the constant control $Q_{\rm ODE}^{\rm FB,opt}$ is used in system (1),(10)-(12) the bioreactor is driven to washout (see Definition

2.1) before the decontamination target is achieved. These results seem to show that when high diffusions are considered, the optimal controls obtained with the ODE and ODE-PDE models are similar, whereas for low diffusion coefficients the ODE-PDE model exhibits better results, in the sense that it provides smaller volumetric flow rates that favor that the biomass does not become extinct before the target is achieved.

- **Nonhomogeneous flow velocity field**: In order to analyze the similarities between the obtained optimal controls $Q_{\text{ODE}}^{\text{FB,opt}}$, $Q_{\text{NH}}^{\text{FB,opt}}$ and $Q_{\text{NH}}^{\text{OL,opt}}(\Sigma)$, we plot them in Figure 8. It is easy to observe that the volumetric flow rates $Q_{\text{NH}}^{\text{FB,opt}}$ and $Q_{\text{NH}}^{\text{OL,opt}}(\Sigma)$, obtained with the ODE-PDE system (1),(10)-(12) when $\tau_{\text{b}} \ll \tau_{\text{r}}$ and $\tau_{\text{b}} \approx \tau_{\text{r}}$, are respectively around 75% and 35% the value of the flux $Q_{\text{ODE}}^{\text{FB,opt}}$. As a result we can conclude that the ODE-PDE systems exhibits better results when computing the optimal feedback, in the sense that it provides smaller volumetric flow rates that favor that the biomass does not become extinct before the target is achieved.

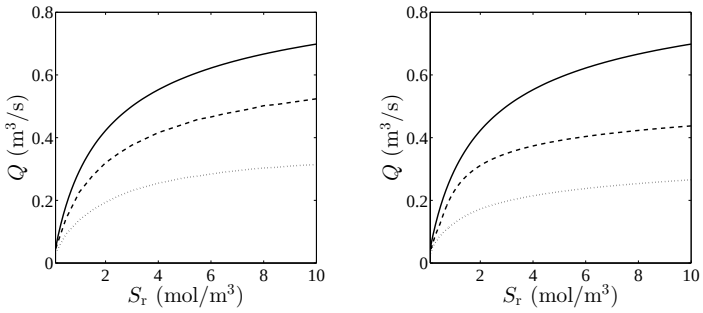


(a) $Q_{\text{ODE}}^{\text{FB,opt}}$ vs $Q_{\text{H}}^{\text{FB,opt}}$ (b) $Q_{\text{ODE}}^{\text{FB,opt}}$ vs $Q_{\text{H}}^{\text{OL,opt}}(\Sigma)$

Figure 7: Homogeneous flow velocity field: Comparison between the feedback obtained for the ODE model (depicted with solid line), the feedback obtained for the ODE-PDE model when $\tau_{\text{b}} \ll \tau_{\text{r}}$ (depicted with dashed lines) and the feedback obtained for the ODE-PDE model when $\tau_{\text{b}} \approx \tau_{\text{r}}$ (depicted with dotted lines).

Comparison between the considered control strategies

Here, we compare the open-loop and feedback controls obtained in Sections 4.2.2 and 4.3.2. From Tables 6 and 8, one can observe that the decontamination times obtained using time-varying open loops and feedbacks are similar. However, the feedback approximation exhibits two advantages with respect to time-dependent controls: it is more robust to possible changes on the system conditions and, once obtained, it can be applied in other scenarios without additional computational cost. Finally, one can see that the decontamination times



(a) $Q_{\text{ODE}}^{\text{FB,opt}}$ vs $Q_{\text{NH}}^{\text{FB,opt}}$ (b) $Q_{\text{ODE}}^{\text{FB,opt}}$ vs $Q_{\text{NH}}^{\text{OL,opt}}(\Sigma)$

Figure 8: Nonhomogeneous flow velocity field: Comparison between the feedback obtained for the ODE model (depicted with solid line), the feedback obtained for the ODE-PDE model when $\tau_b \ll \tau_b$(depicted with dashed lines) and the feedback obtained for the ODE-PDE model when $\tau_b \approx \tau_r$ (depicted with dotted lines).

among constant controls are twice larger than those among time-varying open loops and feedbacks.

5. Conclusion

In this work, we have focused on the modeling of the problem of water treatment by using continuous bioreactors. We have presented two mathematical models, assuming homogeneity or inhomogeneity of substrate and biomass concentrations in the bioreactor. We have also made a difference between considering that the fluid flow velocity in the bioreactor is homogeneous through the inlet, or follows a nonhomogeneous profile.

We have tackled an optimization problem which aims to minimize the time needed to clean the polluted resource, by choosing an optimal bioreactor volumetric inflow rate. In the case of considering homogeneity of the contaminant in the bioreactor, it is possible to obtain analytically an optimal flow rate from previous theoretical results. In the case of considering inhomogeneity of the contaminant in the bioreactor, we show here how to obtain an optimal flow rate using an hybrid genetic algorithm. The results show that, in the cases where the time scale in the bioreactor is comparable with the time scale of the resource (for instance, by using $D_S = D_B = 0.01$ (m^2/s)), the optimal flow rates are smaller than the optimal flow rates obtained for the mathematical model which considers homogeneity in the bioreactor. In any case, the decontamination time can be substantially reduced if feedback controls are used instead of constant controls.

Our goal was to compare the numerical optimization results obtained for the ODE and ODE-PDE models presented for coupled system between the bioreactor and the water resource. The results show that when the time scale of the bioreactor is much smaller than the one of the water resource, (for instance, by

using $D_S = D_B = 100$ (m^2/s)), the ODE-PDE system with homogeneous flow velocity field approaches the ODE system. Contrarily, the ODE-PDE system with nonhomogeneous flow velocity field does not approach the ODE system in the sense that, when using the control strategy that is optimal under the homogeneous assumption in the bioreactor, the biomass becomes extinct and it is not able to make the substrate in the water resource decrease to the objective value. Let us notice that the nonhomogeneous flow velocity field has been presented in order to approach a more realistically behavior of the reactor (see [34]). An important conclusion is that an optimal feedback derived for perfectly mixed bioreactor can lead a bioreactor with non negligible diffusion terms to washout, preventing the desired decontamination objective to be reached, while a simple open loop control, obtained with the method presented in this work, can solve the problem.

Acknowledgements

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