OPTIMAL CONTROL APPLICATIONS & METHODS
Optim. Control Appl. Meth., **20**, 145–164 (1999)

OPTIMAL TIME CONTROL OF BIOREACTORS FOR THE WASTEWATER TREATMENT

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SUMMARY

In this work the time optimal control problem for a biological sequencing batch reactor, used for wastewater treatment, is solved. This operation strategy increases greatly the efficiency of these plants. New is the consideration of the substrate concentration in the input flow, the main disturbance for these systems, as a variable signal and not as a constant parameter. The problem will be solved using a known method based on Green's theorem that allows one to obtain analytically the unique global solution. Furthermore, an optimal feedback control law can be derived that can be made robust against parameter uncertainties and the input disturbance. Simulations of a realistic model of an industrial wastewater treatment plant show the advantages of using an optimal strategy in the control of the plant, since this reduces, among other aspects, the costs of operation and the size of the plant. Copyright © 1999 John Wiley & Sons, Ltd.

KEY WORDS: time optimal control; non-linear systems; biological reactors; robust feedback control

1. INTRODUCTION

Activated sludge is an aerobic biological process in which wastewater is mixed with a suspension of microorganisms to assimilate pollutants and is then settled to separate the treated effluent. It has been traditionally applied in continuous flow processes with fixed volume tanks. The treatment of industrial wastewaters by the activated sludge process is common, but the nature of many industrial discharges often cause operational problems in continuous flow systems. Sequencing batch reactors (SBR) offer a number of advantages over continuous flow systems.[1] They offer for example greater flexibility in control strategy and to be effective they require fully automated computer controls.

In general the SBR process is distinguished by three major characteristics: periodic repetition of a sequence of well-defined process phases; planned duration of each process phase in accordance with the treatment result to be met; progress of the various biological and physical reactions in time rather than in space.

In the SBR system all treatment takes place in a single reactor with different phases separated in time. The cycle in a typical SBR is divided into five discrete time periods: *Fill*, *React*, *Settle*, *Draw*, and *Idle*. At the beginning of each cycle, the SBR contains a certain volume of water, and activated sludge settled at the bottom of the reactor. The cycle starts with a fill phase of distinct duration. The fill phase may be short or long depending on the effects which are desired to be achieved.

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Contract/grant sponsor: DGAPA, UNAM, Mexico; Contract/grant number: PAPIIT IN118098

CCC 0143–2087/99/030145–20$17.50

Received 25 November 1997
Revised 23 March 1999

With the beginning of the fill phase, or some time later, the aerator is turned on. The reaction (or aeration) phase which now begins may last until the biodegradable portion of the organic wastewater constituents has been degraded. Mixer and aerator are turned off for the settle phase. The sludge is allowed to settle under entirely quiescent conditions. A clear water zone (supernatant) appears which can be progressively withdrawn as the sludge blanket moves downwards. When the low operating level is reached the draw is stopped. Excess solids are withdrawn from the bottom at the end of the draw phase. The reactor then enters the idle phase which continues until the beginning of the next cycle.

A reduction of the cycle time of the SBR increases the quantity of pollutants that can be treated by the process. As the settle, draw and idle phases are usually of fixed time or not controllable by the operator, the cycle time of the SBR can be only reduced if the fill and reaction times can be reduced. A simplified model of these phases (see (1)) can be easily obtained using mass balance equations.[2,3] The obtained model has three state and one control variables. In this paper this model will be taken as the basis to find the best strategy for the control variable in the sense that the total time of the fill and reaction phases will reach a minimum. Such problems are usually solved using the Maximum Principle of Pontryagin of the Optimal Control Theory.[4,5] This principle provides a set of necessary conditions that have to be satisfied by the optimal control law. In this paper an alternative method due to Miele,[6] based on Green's theorem, and suited for plane systems, will be used for solving this problem. For that purpose an equivalent plane description of the original three-state model has to be found. This is done after a controllability analysis of the original system. An advantage of this method is that it is a global approach to minimization, i.e. does not depend on local approximations as does the maximum principle. Furthermore, for singular arcs, where the maximum principle yields no constructive information, Green's method can solve the problem.

Optimal problems have been solved for biological reactors for other purposes, specially in biotechnology.[3] In References 7 and 8, the Green's method has been used to optimize the transient of a continuous reactor. In Reference 9 the feed rate was considered as a control variable of a fed batch fermenter and an analytic expression for the switching times between bang–bang control intervals and singular arcs was derived. The objective was the maximization of the product output. General characteristics for the optimal feed rate profiles for different classes of fed batch fermentations were presented in Reference 10, and in Reference 11 these characteristics were used to establish a numerical procedure. In Reference 12 the substrate concentration in the fermenter was used as the control variable to derive a non-singular control problem. A numerical procedure to solve optimization problems in batch fermentation is proposed in Reference 13. In Reference 14 a numerical optimization procedure is presented to optimize fed batch fermenters in the presence of uncertainty in the model parameters. In References 15 and 16 a methodology is introduced to derive easy-to-implement adaptive controllers from optimal control solutions for fermentation processes.

In all these works the substrate concentration at the input flow (S_{in}) is considered as a constant. Whereas this is possible in biotechnological processes, since this concentration can be controlled, for wastewater treatment processes this variable is one of the most important disturbances and cannot be considered either as a constant nor as a control variable. The main objectives of this article are: (1) To determine rigorously (i.e. necessary and sufficient conditions) the optimal feeding policy for a fed batch bioreactor for the wastewater treatment. Green's method will be used for this purpose. A contribution in this aspect is the consideration of varying substrate concentration in the input flow , which is an important disturbance. Analytical expressions are derived and the interest is not in a numerical procedure. This leads to an understanding of the fundamental features of the optimal strategy, that is not possible by numerical solutions.

(2) A feedback control law will be found that solves the optimal problem for different initial conditions. (3) A robust feedback control law will be given that is almost optimal and is robust against some disturbances and parameter uncertainties in the model of the plant.

2. SYSTEM DESCRIPTION AND PROBLEM FORMULATION

The reactor can be described by the following set of ordinary differential equations:

$$\begin{aligned} \dot{X}(t) &= \left(\mu(S(t)) - \frac{F_{\text{in}}(t)}{V(t)} \right) X(t) \\ \dot{S}(t) &= -\frac{1}{Y}\,\mu(S(t))X(t) + \frac{F_{\text{in}}(t)}{V(t)}\,(S_{\text{in}}(t) - S(t)) \\ \dot{V}(t) &= F_{\text{in}}(t), \end{aligned} \tag{1}$$

where

X	biomass concentration in the tank, $\mathrm{M\,L^{-3}}$
S	substrate concentration in the tank, $\mathrm{M\,L^{-3}}$
V	volume of water in the tank, $\mathrm{L^3}$
$\mu(S)$	specific growth rate, $\mathrm{T^{-1}}$
F_{in}	input water flow to the tank, $\mathrm{L^3\,T^{-1}}$
Y	yield coefficient,
S_{in}	substrate concentration in the input flow, $\mathrm{M\,L^{-3}}$

F_{in}, the control variable, can only take values in a positive and closed interval $F_{\text{in}} \in [0, F_{\max}]$, $F_{\max} > 0$, and all three state variables (X, S, V) have to be positive, i.e. $X \geqslant 0$, $S \geqslant 0$ and $V \geqslant 0$. Furthermore to make the description physically meaningful it will be assumed that after a maximum level of water in the tank $V_{\max}$ has been reached the input flow F_{in} is automatically turned off to avoid overflow. It will be also assumed that Y is *constant* and that $\mu(S)$ is defined for $S \geqslant 0$, $\mu(0) = 0$, is positive (i.e. $\mu(S) > 0$ for $S > 0$), bounded (i.e. $\mu(S) \leqslant M$ for every $S > 0$ and for some positive constant M), and is once continuously differentiable. S_{in} will be considered not as a constant but as a variant quantity and $S_{\text{in}}(t) \geqslant 0$.

The objective of such a reactor is to bring the concentration of the substrate in the tank S under a specified level $S_{\min}$, while the volume is brought from V_0 to V_{f}, where $0 < V_0 < V_{\text{f}} \leqslant V_{\max}$. Usually in practice the concentration of pollutants in the water to be treated is not uniformly distributed, what is reflected in the fact that $S_{\text{in}}(t)$ in model (1) is not constant. For wastewater treatment processes this is in fact one of the main disturbances. We want to deal with the following physically meaningful situation: Consider that the wastewater to be fed to the reactor is contained in a pipeline of volume bigger than $V_{\text{f}} - V_0$, and that the substrate concentration along the pipeline changes arbitrarily (This is only a possible physical interpretation of the mathematical conditions to solve the problem). It is of course of interest to optimize the efficiency of the process, defined as the quantity of substrate treated per unit of time. Since the process is cyclic one has to maximize the efficiency per cycle ε_{c}, given by

$$\varepsilon_{\text{c}} = \frac{\int_0^{T_{\text{c}}} F_{\text{in}}(\tau) S_{\text{in}}(\tau)\,\mathrm{d}\tau + S_0 V_0 - S_{\min} V_{\text{f}}}{T_{\text{c}}},$$

i.e. the quantity of substrate degraded during the cycle divided by T_c, the cycle time (The value of T_c depends on the input function $F_{in}(t)$). If we assume that the shape of the substrate concentration in the pipeline does not change with time, then for every pair of control functions $F^1_{in}(t)$, $F^2_{in}(t)$ that satisfy $\int_0^{t_1} F^1_{in}(\tau)\,d\tau = \int_0^{t_2} F^2_{in}(\tau)\,d\tau$, for some $t_1, t_2 \geqslant 0$, it follows that $\int_0^{t_1} F^1_{in}(\tau) S_{in}(\tau)\,d\tau = \int_0^{t_2} F^2_{in}(\tau) S_{in}(\tau)\,d\tau$. Therefore the numerator of the expression for ε_c is equal for all control inputs that satisfy $\int_0^{T_c} F_{in}(\tau)\,d\tau = V_f - V_0$, and the maximization of ε_c coincides with the minimization of T_c. The cycle time T_c consists of a fixed period T_f, for decantation and emptying the tank, and of the fill and reaction time T_r, which can be controlled.

Therefore it is sought a *state feedback control law* for the input variable F_{in} that brings the system from a given initial state $x_0 = [X_0, S_0, V_0]$ to a final one $x_f = [X_f, S_f, V_f]$, in a set of desired final states $\mathbf{X}_f \doteq \{\mathbf{x}_f | 0 \leqslant S_f \leqslant S_{min}, V_f\}$, in minimal time, using an admissible input function and along an admissible trajectory.

According to the physical conditions of the system an input function is considered admissible if

$$0 \leqslant F_{in} \leqslant F_{max} \tag{2}$$

and a trajectory is also admissible if for every time $t \geqslant 0$ it lies in the region

$$\Omega_A \doteq \{(X, S, V) | X > 0, S \geqslant 0, 0 < V_{min} \leqslant V \leqslant V_{max}\} \tag{3}$$

The case $X = 0$ is excluded because it is not physically interesting (the reactor is 'dead'), and if $X_0 > 0$ it cannot be reached for any input by the system (1). The restrictions for the volume of the tank V come from the fact that the tank cannot be completely emptied and that it has finite physical dimensions.

The cost functional to be minimized is the reaction time T_r, i.e.

$$J[F_{in}] = \int_0^{T_r} d\tau \tag{4}$$

Under the conditions imposed on $S_{in}(t)$ the quantity of substrate input into the tank at any time, i.e. $\int_0^t F_{in}(\tau) S_{in}(\tau)\,d\tau$, depends only on the quantity of water that has been input, i.e. $\int_0^t F_{in}(\tau)\,d\tau = V(t)$, and not on how this is done, i.e. on the form of $F_{in}(\tau)$. Therefore the input quantity of substrate is a function of the volume change

$$\int_0^t F_{in}(\tau) S_{in}(\tau)\,d\tau = W(V(t)) - W(V_0) \tag{5}$$

For simplicity it will be assumed that $W(\cdot)$ is a twice continuously differentiable function of its argument. Differentiating (5) with respect to t it can be seen that $S_{in}(t)$ can be replaced by a function of $V(t)$, i.e.

$$S_{in}(t) = \tilde{S}_{in}(V(t)) = dW(V(t))/dV \tag{6}$$

Note that (6) implies that $W(V)$ is a monotone increasing function of V and that $\tilde{S}_{in}(\cdot)$ is once continuously differentiable. To solve the posed problem it will be useful to introduce new state variables: $z_1 \doteq XV$, the total amount of biomass, $z_2 \doteq SV$, the total amount of substrate, and $z_3 \doteq V$. The dynamics of the system in these new variables is given by

$$\begin{aligned} \dot{z}_1(t) &= \mu(z_2(t)/z_3(t)) z_1(t) \\ \dot{z}_2(t) &= -\frac{1}{Y}\mu(z_2(t)/z_3(t)) z_1(t) + \tilde{S}_{in}(z_3(t)) F_{in}(t) \\ \dot{z}_3(t) &= F_{in}(t) \end{aligned} \tag{7}$$

The corresponding initial and final states and the final set are $\mathbf{z}_0 = [z_{10}, z_{20}, z_{30}] = [X_0 V_0, S_0 V_0, V_0]$; $\mathbf{z}_f = [X_f V_f, S_f V_f, V_f]$; and $\mathbf{Z}_f \doteq \{\mathbf{z}_f | 0 \leqslant z_{2f} \leqslant S_{\min} V_f , z_{3f} = V_f\}$, respectively.

This is a typical time optimal control problem, which is usually solved recalling the Maximum Principle of Pontryagin.[4] In this paper an alternative method based on Green's theorem will be used for solving this problem.[5,6,17,18]

3. CONTROLLABILITY ANALYSIS AND MINIMAL REPRESENTATION OF THE REACTOR

A controllability analysis of the reactor will show that the representation of the controllable part of it is a bidimensional system, simplifying the solution of the posed control problem.

Equation (7) can be written in compact form as

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}) + \mathbf{g}(\mathbf{z}) F_{\text{in}} \tag{8}$$

where $\mathbf{z}^{\mathrm{T}} = [z_1, z_2, z_3]$, and $\mathbf{f}(\mathbf{z})$ and $\mathbf{g}(\mathbf{z})$ are defined by (7). For initial conditions satisfying (3) the solution of (8) is unique and will be denoted by $\phi(t, F_{\text{in}}, \mathbf{z}_0)$, for an admissible input time function F_{in}, and an initial state $\mathbf{z}_0$ in $t_0 = 0$.

Definition 1

The reachable set from $\mathbf{z}_0$ is[19]

$$\mathscr{R}(\mathbf{z}_0) \doteq \{\mathbf{z} \in \mathbf{R}^3 | \mathbf{z}_0 \rightsquigarrow \mathbf{z}\},$$

where $\mathbf{z}_0 \rightsquigarrow \mathbf{z}$ means that there exists an admissible time function F_{in} such that $\mathbf{z} = \phi(t, F_{\text{in}}, \mathbf{z}_0)$, for some finite $t \geqslant 0$.

The following proposition gives some properties of the reachable set for system (7)

Proposition 2

Let $\mathbf{z}_0^{\mathrm{T}} = [X_0 V_0, S_0 V_0, V_0]$ and F_{in} satisfy (3) and (2), respectively. For system (7) the following statements are true:

(i) The surface

$$\sigma(\mathbf{z}_0) \colon V(X + YS) - YW(V) = \rho(\mathbf{z}_0) \tag{9}$$

where $\rho(\mathbf{z}_0) = V_0(X_0 + YS_0) - YW(V_0)$, is *invariant* for every admissible input function F_{in}.

(ii) $\mathscr{R}(\mathbf{z}_0) \subseteq \sigma(\mathbf{z}_0)$.

(iii) For every $t \geqslant 0$, and every admissible F_{in}, the trajectory $\phi(t, F_{\text{in}}, \mathbf{z}_0)$ is such that $X(t) \geqslant 0$, $S(t) \geqslant 0$, and $V(t) \geqslant V_0$. Moreover if $X_0 > 0$ then $X(t) > 0$ and if $X_0 = 0$ then $X(t) = 0$.

Proof. (i) This follows easily from the fact that

$$\nabla\sigma \cdot (\mathbf{f}(\mathbf{z}) + \mathbf{g}(\mathbf{z}) F_{\text{in}}) = 0$$

The expression for surface (9) can be found integrating between 0 and t the equation

$$Y\frac{\mathrm{d}(VS)}{\mathrm{d}t}+\frac{\mathrm{d}(VX)}{\mathrm{d}t}-Y\,\frac{\mathrm{d}V}{\mathrm{d}t}\,\tilde{S}_{\mathrm{in}}(V)=\frac{\mathrm{d}(Y[VS-W(V)]+VX)}{\mathrm{d}t}=0$$

which can be obtained from (7) and (6). It follows that

$$V(t)(X(t)+YS(t))-YW(V(t))=V_0(X_0+YS_0)-YW(V_0)$$

Therefore $\rho(\mathbf{z}_0)=V_0(X_0+YS_0)-YW(V_0)$.

(ii) This follows easily from the definition of the reachability set from $\mathbf{z}_0$.

(iii) $V\geqslant V_0$ is a consequence of $\dot{V}=F_{\mathrm{in}}$ and the restrictions on F_{in}. From the first equation in (1) it is clear that if $X=0\Rightarrow\dot{X}=0$, and therefore the line $X=0$ on $\sigma(\mathbf{z}_0)$ cannot be crossed. So if $X_0\geqslant 0\Rightarrow X(t)\geqslant 0$ for all $t\geqslant 0$. To prove that $S_0\geqslant 0\Rightarrow S(t)\geqslant 0$ for all $t\geqslant 0$ one can take the surface $\sigma_1: S=0$ and its gradient vector $\nabla\sigma_1=[0,1,0]$ and because $\nabla\sigma_1\cdot(\mathbf{f}(\mathbf{z})+\mathbf{g}(\mathbf{z})F_{\mathrm{in}})\geqslant 0$ for all permitted F_{in} and in the region $\Omega_{\mathrm{A}}\cap\sigma_1$, it follows that the velocity vector always points into the region $S>0$ or is tangent to its boundary. Moreover from (7), the non-negativity of S, $\mu(S)$ and the positivity of V it follows that $X(t)$ is a monotonic increasing function and therefore $X_0>0$ implies $X(t)>0$. Furthermore if $X_0=0$ then $X(t)=0$. $\square$

Remark 3

It follows easily from Proposition 2 that the plant (7) is not controllable, i.e. not every pair of points, even in the permitted region (3), can be connected through a trajectory. Given the initial point $\mathbf{z}_0$ all reachable states lie on the surface $\sigma(\mathbf{z}_0)$.

Remark 4

As an important consequence of Proposition 2 one has that the optimization problem is not well posed because of the lack of controllability of the plant. For the problem to make sense, if the initial state $\mathbf{x}_0=[X_0,S_0,V_0]$ is given, then the final state $x_{\mathrm{f}}=[X_{\mathrm{f}},S_{\mathrm{f}},V_{\mathrm{f}}]$ has to be on the surface $\sigma(\mathbf{z}_0)$ (9). In other words, if $\mathbf{x}_0$ is given, only two components of $\mathbf{x}_{\mathrm{f}}$ can be arbitrarily chosen, and the third one will be determined by the surface $\sigma(\mathbf{z}_0)$. So for example if $[S_{\mathrm{f}},V_{\mathrm{f}}]$ are selected, $\mathbf{X}_{\mathrm{f}}$ has to be chosen to satisfy (9).

Remark 5

The existence of the invariant surface $\sigma(\mathbf{z}_0)$ for the system is a direct consequence of the conservation of mass in the biological reactor: the ongoing mass of substrate is converted in cellular mass or it accumulates in the tank. If there would be a decaying term in the balance of X in (7), the balance equations (7) would not reflect this conservation of mass, and therefore there would not exist the invariant surface $\sigma(\mathbf{z}_0)$.

Remark 6

It follows from Proposition 2 that the set

$$\Omega(\mathbf{z}_0)\doteq\{\mathbf{z}\in\mathbf{R}^3\,|\,\mathbf{z}\in\sigma(\mathbf{z}_0)\wedge X>0\wedge S\geqslant 0\wedge V_{\min}\leqslant V\}\tag{10}$$

is also invariant.

Proposition 2 shows that if an initial state $\mathbf{z}_0$ is given, the dynamics of the system evolves on the two dimensional surface $\sigma(\mathbf{z}_0)$. One can therefore find a representation of the dynamics of the plant on this surface.

Proposition 7

Let $\mathbf{z}_0$ be a given initial state for the system (7) and let $\Omega(z_0)$ be the invariant set defined by (10). Then the dynamics on $\Omega(\mathbf{z}_0)$ of the plant (7) can be described by a set of two ordinary differential equations and an algebraic equation

$$\begin{aligned}
\dot{S} &= -\frac{1}{Y}\,\mu(S)(Y(W(V)/V - S) + \rho(z_0)/V) + \frac{\tilde{S}_{\mathrm{in}}(V) - S}{V}\,F_{\mathrm{in}} \\
\dot{V} &= F_{\mathrm{in}} \\
X &= Y(W(V)/V - S) + \rho(z_0)/V
\end{aligned} \tag{11}$$

Proof. From (9) one can obtain the third equation of (11) and replacing it in (1) the rest of (11) will follow. □

The differential equations of (11) will be written in short form as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})F_{\mathrm{in}} \tag{12}$$

where $\mathbf{x}^{\mathrm{T}} = [S, V]$, and $\mathbf{f}(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$ are defined by (11). For initial conditions in (10) the solution of (12) is unique and will be denoted by $\phi(t, F_{\mathrm{in}}, \mathbf{x}_0)$, for an admissible input time function F_{in} and an initial state $\mathbf{x}_0$ in $t_0 = 0$.

The admissible region $\Omega_{\mathrm{A}}(\mathbf{z}_0)$ for the state vector $\mathbf{x}$ of (11) is the intersection of the admissible set Ω_{A} for the original description of the system (3) and the surface $\sigma(\mathbf{z}_0)$ (9):

$$\Omega_{\mathrm{A}}(\mathbf{z}_0) \doteq \{(S, V) | (0 < V_{\min} \leqslant V \leqslant V_{\max}), (S \geqslant 0), (S < W(V)/V + \rho(\mathbf{z}_0)/(YV))\} \tag{13}$$

4. TIME OPTIMAL CONTROL IN THE PLANE: USE OF GREEN'S THEOREM

The time optimal problem for system (7) can be now (equivalently) reformulated as a time optimal problem for the plane system (11) (or (12)):

Time optimal control problem (*OP*): Let a surface $\sigma(\mathbf{z}_0)$ (9) together with the admissible set $\Omega_{\mathrm{A}}(\mathbf{z}_0)$ (13) be given. Let $\mathbf{x}_0 \in \Omega_{\mathrm{A}}(\mathbf{z}_0)$ be an initial point and $\mathbf{X}_{\mathrm{f}} \doteq \{\mathbf{x}_{\mathrm{f}} | 0 \leqslant S_{\mathrm{f}} \leqslant S_{\min}, V_{\mathrm{f}}\} \subset \Omega_{\mathrm{A}}(\mathbf{z}_0)$ be a set of final states for the system (12). Find an admissible control function F_{in}, to which corresponds an admissible trajectory $\phi(t, F_{\mathrm{in}}, \mathbf{x}_0)$, such that F_{in} transfers $\mathbf{x}_0$ to a point in $\mathbf{X}_{\mathrm{f}}$ in minimal time, i.e. $J[F_{\mathrm{in}}]$ in (4) will be minimized.

For some kinds of optimal problems in the plane Miele[6,17,18] introduced a solution method based on Green's theorem. The method consists essentially in three steps:

1. Determination of the attainable set for the problem, i.e. the region of the plane where the trajectory path of a possible solution should lie.
2. By using Green's theorem the relative optimality of any two possible trajectories in the attainable set can be determined without knowledge of the solutions of the differential

equations, which describe the system. This permits the determination of the optimal trajectory.

3. Once the optimal trajectory has been determined the last step consists in determining an *admissible* control function (here F_{in}), which leads to a solution of the system equations with a trajectory arc which coincides with the optimal path found.

These steps will be further clarified in this section for the concrete time optimal problem (4). The results in the references cannot be applied directly to the present problem but the technique can be adapted to solve it.

4.1. Attainable set for the time optimal problem

Given an initial point $\mathbf{x}_0$ and a set of final states $\mathbf{X}_{\mathrm{f}} \doteq \{\mathbf{x}_{\mathrm{f}} | 0 \leqslant S_{\mathrm{f}} \leqslant S_{\min}, V_{\mathrm{f}}\}$, both in $\Omega_{\mathrm{A}}(\mathbf{z}_0)$, if a solution to the optimal control problem exists, the segment of the trajectory connecting $\mathbf{x}_0$ to $\mathbf{x}_{\mathrm{f}} \in \mathbf{X}_{\mathrm{f}}$ must lie in $R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}})$, where

$$R(\mathbf{x}_0) \doteq \{\mathbf{x} \in \Omega_{\mathrm{A}}(\mathbf{z}_0) | x = \phi(t, F_{\mathrm{in}}, x_0), \text{ for some } t \in [0, \infty), F_{\mathrm{in}} \text{ admissible}\}$$

$$R(\mathbf{X}_{\mathrm{f}}) \doteq \{x \in \Omega_{\mathrm{A}}(\mathbf{z}_0) | \exists\, \mathbf{x}_{\mathrm{f}} \in \mathbf{X}_{\mathrm{f}},\ \mathbf{x}_{\mathrm{f}} = \phi(t, F_{\mathrm{in}}, x), \text{ for some } t \in [0, \infty), F_{\mathrm{in}} \text{ admissible}\}$$

i.e. $R(\mathbf{x}_0)$ is the set of points in $\Omega_{\mathrm{A}}(\mathbf{z}_0)$ which can be attained from $\mathbf{x}_0$ and $R(\mathbf{X}_{\mathrm{f}})$ denotes the set of points in $\Omega_{\mathrm{A}}(\mathbf{z}_0)$ from which one point in $\mathbf{X}_{\mathrm{f}}$ can be attained. Alternatively $R(\mathbf{X}_{\mathrm{f}})$ can be defined as

$$R(\mathbf{X}_{\mathrm{f}}) \doteq \{\mathbf{x} \in \Omega_{\mathrm{A}}(\mathbf{z}_0) | \exists\, \mathbf{x}_{\mathrm{f}} \in \mathbf{X}_{\mathrm{f}},\ \mathbf{x} = \phi(-t, F_{\mathrm{in}}, \mathbf{x}_{\mathrm{f}}), \text{ for some } t \in [0, \infty), F_{\mathrm{in}} \text{ admissible}\},$$

with $\phi(-t, F_{\mathrm{in}}, \mathbf{x}_{\mathrm{f}})$ the solution of

$$\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x}) - \mathbf{g}(\mathbf{x}) F_{\mathrm{in}}, \quad \mathbf{x}(0) = \mathbf{x}_{\mathrm{f}}$$

On the other side if $R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}}) \neq \emptyset$, the empty set, then there is an admissible control F_{in} such that an arc of the trajectory $\phi(t, F_{\mathrm{in}}, x_0)$ joints $\mathbf{x}_0$ and some $\mathbf{x}_{\mathrm{f}} \in \mathbf{X}_{\mathrm{f}}$. This is the question on the existence of a solution to the optimal problem.

It will be shown that in the present case the set $R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}})$ is delimited by the trajectories $\phi(t, F_{\max}, \mathbf{x}_0)$, $\phi(t, 0, \mathbf{x}_0)$ and $\phi(-t, 0, \mathbf{x}_{\mathrm{f}}^{\mathrm{T}} = [0, V_{\mathrm{f}}])$ and the segment $S = 0$, $V_0 \leqslant V \leqslant V_{\mathrm{f}}$. Figure 1 illustrates this region.

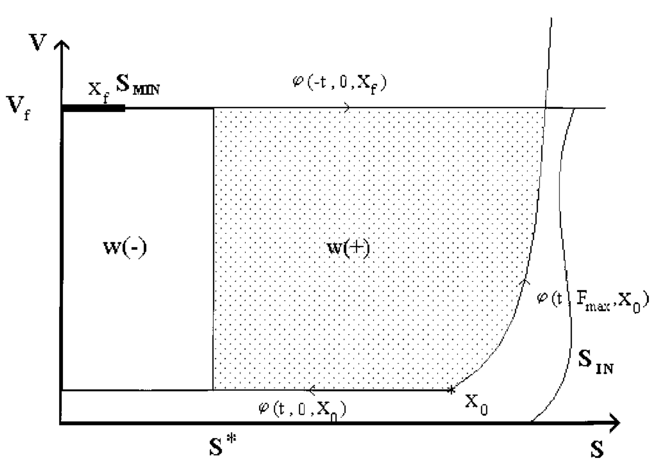

Figure 1. Admissible set (shaded) and sign of the function ω of Green's theorem

Proposition 8

Let $\mathbf{x}_0^{\mathrm{T}} = [S_0, V_0] \in \Omega_{\mathrm{A}}(\mathbf{z}_0)$ and $\mathbf{X}_{\mathrm{f}} = \{\mathbf{x}_{\mathrm{f}} | 0 \leqslant S_{\mathrm{f}} \leqslant S_{\min}, V_{\mathrm{f}}\} \subset \Omega_{\mathrm{A}}(\mathbf{z}_0)$ be given, such that $S_{\min} > 0$, and $V_0 < V_{\mathrm{f}} \leqslant V_{\max}$. Let $\bar{\mathscr{S}}$ be the compact simply connected set bounded by the arcs $\phi(t, F_{\max}, \mathbf{x}_0)$, $\phi(t, 0, \mathbf{x}_0)$ and $\phi(-t, 0, \mathbf{x}_{\mathrm{f}}^{\mathrm{T}} = [0, V_{\mathrm{f}}])$ and the segment $\lambda = \{(S, V) | S = 0, V_0 \leqslant V \leqslant V_{\mathrm{f}}\}$. Let also $\mathscr{S} \doteq \bar{\mathscr{S}} \setminus \lambda$, i.e. $\mathscr{S}$ is the set $\bar{\mathscr{S}}$ without the left boundary (see Figure 1). Then $\mathscr{S} = R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}})$ and its interior is not empty.

Proof. Note that since $X_0 > 0$ then $S(t) < \rho(\mathbf{z}_0)/YV(t) + W(V(t))/V(t)$ for every $F_{\mathrm{in}}(t)$ and $t \geqslant 0$. Let us describe first the three trajectories that define $\mathscr{S}$:

(1) $\phi(t, 0, \mathbf{x}_0)$: $V(t) = V_0$ and $\dot{S} = -\mu X/Y$, i.e. V is constant and S tends asymptotically to $S = 0$, when t goes to ∞. Therefore λ is not reached in finite time.
(2) $\phi(-t, 0, \mathbf{x}_{\mathrm{f}})$: $V(t) = V_{\mathrm{f}}$ and $\dot{S} = \mu X/Y$, i.e. V is constant, S grows monotonically and asymptotically towards $S = \rho(\mathbf{z}_0)/YV_{\mathrm{f}} + W(V_{\mathrm{f}})/V_{\mathrm{f}}$ (i.e. $X = 0$).
(3) $\phi(t, F_{\max}, x_0)$: $V(t) = V_0 + F_{\max} t$, i.e. V grows monotonically and $0 < S < \rho(\mathbf{z}_0)/YV_{\mathrm{f}} + W(V_{\mathrm{f}})/V_{\mathrm{f}}$. Therefore this trajectory intersects the line $V = V_{\mathrm{f}}$ at a unique point $0 < \hat{S} < \rho(\mathbf{z}_0)/YV_{\mathrm{f}} + W(V_{\mathrm{f}})/V_{\mathrm{f}}$.

Now let us prove the proposition:

(a) Assume $\mathbf{y} \notin \mathscr{S}$. It will be shown that $y \notin R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}})$. Write $\mathbf{y} \neq (S_y, V_y)$. There are four possibilities for $\mathbf{y}$ to be outside $\mathscr{S}$. Let us consider each case:

1. $\mathbf{y}$ is to the left of $S = 0$, i.e. $S_y \leqq 0$. From Proposition 2 and the preceding discussion it follows that $\mathbf{y} \notin R(\mathbf{x}_0)$.
2. $\mathbf{y}$ is over the line $V = V_{\mathrm{f}}$, i.e. $V_y > V_{\mathrm{f}}$. Since $\dot{V} \geqslant 0$ it follows that $\mathbf{y} \notin R(\mathbf{X}_{\mathrm{f}})$.
3. $\mathbf{y}$ is under the line $V = V_0$, i.e. $V_y < V_0$. Since $\dot{V} \geqslant 0$ it follows that $\mathbf{y} \notin R(\mathbf{x}_0)$.
4. $\mathbf{y}$ is to the right of the arc $\phi(t, F_{\max}, \mathbf{x}_0)$. In this case it happens that $y \notin R(\mathbf{x}_0)$. To show this note that the only possibility to reach y from $\mathbf{x}_0$ is crossing the arc $\phi(t, F_{\max}, \mathbf{x}_0)$, since this trajectory goes to infinity for big t and no trajectory can go around $\mathbf{x}_0$ under the line $V = V_0$. To cross the arc $\phi(t, F_{\max}, \mathbf{x}_0)$ it is necessary that the velocity vector $\dot{\mathbf{x}}$ for some F_{in} at some point on the arc points to the right of it. But this is not possible because the velocity vector for any F_{in} is always between the corresponding vectors for $F_{\mathrm{in}} = 0$ and $F_{\mathrm{in}} = F_{\max}$, and the velocity vector for $F_{\mathrm{in}} = 0$ points always to the left of the arc $\phi(t, F_{\max}, \mathbf{x}_0)$ for any point in $\mathscr{S}$.

(b) Assume $\mathbf{y} \in \mathscr{S}$. It will be shown that $\mathbf{y} \in R(\mathbf{x}_0) \cap R(\mathbf{X}_{\mathrm{f}})$. If $\mathbf{y} = (S_y, V_y)$ then the following control strategy will always steer $\mathbf{x}_0$ to $\mathbf{y}$: make $F_{\mathrm{in}} = F_{\max}$ until the line $V = V_y$ is reached (this occurs in finite time), and then change to $F_{\mathrm{in}} = 0$ until $\mathbf{y}$ has been reached. Therefore $\mathbf{y} \in R(\mathbf{x}_0)$. The following control strategy always steers $\mathbf{y}$ to $\mathbf{X}_{\mathrm{f}}$: make $F_{\mathrm{in}} = F_{\max}$ until the line $V = V_{\mathrm{f}}$ is reached, and then change to $F_{\mathrm{in}} = 0$ until $\mathbf{X}_{\mathrm{f}}$ has been reached. Since $V_{\mathrm{f}} > V_0$ and $S_{\mathrm{in}} > 0$ then it is clear that the interior of $\mathscr{S}$ is not empty. □

Proposition 9

Under the hypothesis of Proposition 8 there exists a solution to the time optimal control problem (OP).

Proof. This follows easily from standard results on existence of optimal controllers. See for example[5] (Corollary 2, Section 4.2). □

4.2. Synthesis of the optimal trajectory by Green's theorem

For a given trajectory arc $\phi(\cdot, F_{in}, \cdot)$ connecting two points P_0 and $P_1 \in \mathscr{S}$, the functional $J[F_{in}]$ (4) can be expressed as a line integral along this arc. To see why, note first that $\Delta(\mathbf{x}) = -\det[\mathbf{f}(\mathbf{x}), \mathbf{g}(\mathbf{x})] = \mu X/Y \neq 0,\ \forall \mathbf{x} \in \mathscr{S}$. Furthermore the function $\Delta(\mathbf{x})$ can be transformed to

$$\begin{aligned}\Delta(x) &= -\det[\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})F_{in}, \mathbf{g}(\mathbf{x})] \\ &= -\det[\dot{\mathbf{x}}, \mathbf{g}(\mathbf{x})] = \dot{x}_2 g_1(\mathbf{x}) - \dot{x}_1 g_2(\mathbf{x})\end{aligned} \tag{14}$$

Therefore the functional $J[F_{in}]$ (4) can be rewritten as

$$J[F_{in}, P_0, P_1] = \int_0^{T_r} d\tau = \int_0^{T_r} \frac{\dot{x}_2 g_1(\mathbf{x}) - \dot{x}_1 g_2(\mathbf{x})}{\Delta(\mathbf{x})} d\tau = \int_{P_0}^{P_1} \left(\frac{g_1(\mathbf{x})}{\Delta(\mathbf{x})} dx_2 - \frac{g_2(\mathbf{x})}{\Delta(\mathbf{x})} dx_1 \right)$$

i.e. as a line integral along the arc $\phi(\cdot, F_{in}, \cdot)$.

Now suppose that there are two different trajectories $\phi(\cdot, F_{in}, \cdot)$ and $\phi(\cdot, F^*_{in}, \cdot)$, both joining P_0 to P_1 in $\mathscr{S}$, and having no points other than P_0 and P_1 in common. Let Γ be the closed curve formed by these trajectory arcs. If Γ is traversed in counterclockwise direction by following first the arc of $\phi(\cdot, F_{in}, \cdot)$ from P_0 to P_1 and next the arc of $\phi(\cdot, F^*_{in}, \cdot)$ from P_1 to P_0, then the difference of the functional values of the trajectories

$$J[F_{in}, P_0, P_1] - J[F^*_{in}, P_0, P_1] = \oint_\Gamma \left(\frac{g_1(\mathbf{x})}{\Delta(\mathbf{x})} dx_2 - \frac{g_2(\mathbf{x})}{\Delta(\mathbf{x})} dx_1 \right) \tag{15}$$

is a measure of the relative optimality of the two trajectories, i.e. if the difference is positive the trajectory $\phi(\cdot, F^*_{in}, \cdot)$ is better than $\phi(\cdot, F_{in}, \cdot)$, and vice versa.

Since the bounding curve Γ is a Jordan curve, applying Green's Theorem (This is permissible because $\mathbf{f}$ and $\mathbf{g}$ are once continuously differentiable functions in $\mathscr{S}$), i.e.

$$\oint_\Gamma u\, dy + v\, dx = \iint_R \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) dx\, dy = \iint_R \omega(x, y)\, dx\, dy$$

to (15) the following result is obtained:

$$J[F_{in}, P_0, P_1] - J[F^*_{in}, P_0, P_1] = \iint_\Phi \omega(\mathbf{x})\, ds \tag{16}$$

where

$$\omega(\mathbf{x}) = \frac{\partial}{\partial x_1} \left(\frac{g_1(x)}{\Delta(x)} \right) + \frac{\partial}{\partial x_2} \left(\frac{g_2(x)}{\Delta(x)} \right) \tag{17}$$

and Φ is the region enclosed by Γ. Since $\omega(\mathbf{x})$ is uniquely determined for all $\mathbf{x} \in \mathscr{S}$ and can be calculated without solving the differential equation (12), then (16) provides a direct means for determining the optimal strategy. This has to be done for each concrete case. In next section this will be pursued for some concrete situations of the wastewater treatment reactors.

4.3. Determination of the optimal control function

The determination of the optimal trajectory for the problem (OP) is carried out by comparing the relative optimality for all possible admissible trajectories in the admissible set using Green's theorem. The next step consists in finding a control function $\hat{F}_{in}$ leading to the optimal trajectory, i.e. $\phi(t, \hat{F}_{in}, \mathbf{x}_0)$ is the optimal trajectory. For most of the cases it is easy to find such a control function, so that this issue will not be further discussed.

If there is a control function which realizes the optimal trajectory two important questions are if this control function is *unique* and if it is *admissible*. The uniqueness (within a set of measure zero) of the control function is assured if the function $\Delta(\mathbf{x})$ is different from zero along the trajectory, i.e. $\Delta(\mathbf{x}) \neq 0$ for $\mathbf{x} \in \phi(t, \hat{F}_{in}, \mathbf{x}_0)$ (see References 17 and 18).

It may happen that the optimal trajectory can be realized by a control function F_{in} in a unique manner but that this function is not admissible, i.e. F_{in} does not satisfy the restrictions imposed on it. In this case the solution is not valid and the method is inconclusive. It is therefore important to assure for each case that the admissibility condition on the control function is satisfied.

5. TIME OPTIMAL STRATEGY FOR THE BIOLOGICAL REACTOR

In this section the method described in the last one will be applied to the time optimal problem for the biological reactor (11). Since the solution depends in general of the form of the specific growth rate $\mu(S)$, some important and usual descriptions of this function will be considered and the solution of the optimal problem for them will be found. Since we are interested not only in an 'open loop' solution, i.e. to find a function F_{in} which solves the optimal problem, a *feedback law*, which solves the problem, will be given.

For the system (11) the function $\omega(\mathbf{x})$ defined in (17) can be found to be

$$\omega(\mathbf{x}) = -\frac{\mathrm{d}\mu(S)}{\mathrm{d}S}\frac{Y(\tilde{S}_{in}(V) - S)}{\mu^2(S)VX} \tag{18}$$

The sign of ω in $R(\mathbf{x}_0) \cap R(\mathbf{X}_f)$ depends essentially on the signs of $\mathrm{d}\mu/\mathrm{d}S$ and $(\tilde{S}_{in}(V) - S)$, because the denominator of (18) is always positive in this region. The following results are given only for the case when the trajectories lie in the region $S \leqslant \tilde{S}_{in}(V)$, since then the integral (16) does not have to be evaluated explicitly and its sign is sufficient information for the determination of the optimal path. Therefore it will be assumed

(H1) For system (11) $\mathbf{x}_0$ is such that $X_0 > 0$, and $\tilde{S}_{in}(V(t)) - S(t) \geqslant 0$ for $t \geqslant 0$ and $V(t) \leqslant V_f$, where $V(t)$ and $S(t)$ correspond to the trajectory $\phi(t, F_{max}, \mathbf{x}_0)$.

If (H1) is not satisfied the optimal control law can be calculated integrating (16) explicitly. That (H1) is satisfied will depend in general on the parameters of the system, the form of $\tilde{S}_{in}(V)$ and the initial conditions. The following lemma gives some sufficient conditions for (H1) to be fulfilled independently of the parameters of the system:

Lemma 10

For system (11) suppose that $\mathbf{x}_0$ is such that $X_0 > 0$, $\tilde{S}_{in}(V_0) - S_0 \geqslant 0$, that $\tilde{S}_{in}(V)$ is differentiable and $\mathrm{d}\tilde{S}_{in}(V)/\mathrm{d}V \geqslant 0$ for $V_0 \leqslant V \leqslant V_f$, then $\tilde{S}_{in}(V(t)) - S(t) \geqslant 0$ for $t \geqslant 0$ and $V(t) \leqslant V_f$ for every admissible $F_{in}(t)$.

Proof. Set $e \doteq \tilde{S}_{in}(V) - S$. Therefore $\dot{e} = -F_{in}e/V + \mu(S)X/Y + \tilde{S}'_{in}(V)F_{in}$ and it can be easily seen that if $e(0) = \tilde{S}_{in}(V_0) - S_0 \geqslant 0$ and $\tilde{S}'_{in}(V) \geqslant 0$ then $e(t) = \tilde{S}_{in}(V(t)) - S(t) \geqslant 0$ for $t \geqslant 0$. $\square$

In particular if $S_{\mathrm{in}}(t)$ is constant the conditions of the lemma are satisfied. Two cases for the form of the specific growth rate $\mu(S)$ will be considered: monotonic $\mu(S)$ (Monod law); and non-monotonic $\mu(S)$ with just one maximum point (Haldane model).

5.1. Monotonic $\mu(S)$ (Monod law)

In this case $\mu(S)$ is characterized by the fact that $\mathrm{d}\mu/\mathrm{d}S > 0$ for every $S \geqslant 0$. A typical expression is the Monod law (see Figure 2) given by

$$\mu(S) = \frac{\mu_0 S}{K_s + S} \tag{19}$$

where K_s ($\mathrm{M\,L^{-3}}$) is the Monod constant and μ_0 ($\mathrm{T^{-1}}$) the maximum specific growth rate. This model is appropriate when the substrate does not inhibit the activity of the biomass.

Theorem 11

Let $\mu(S)$ be positive (i.e. $\mu(S) > 0$ for $S > 0$), $\mu(0) = 0$, bounded (i.e. $\mu(S) \leqslant M$ for every $S > 0$ and for some positive constant M), once continuously differentiable, and strictly monotone

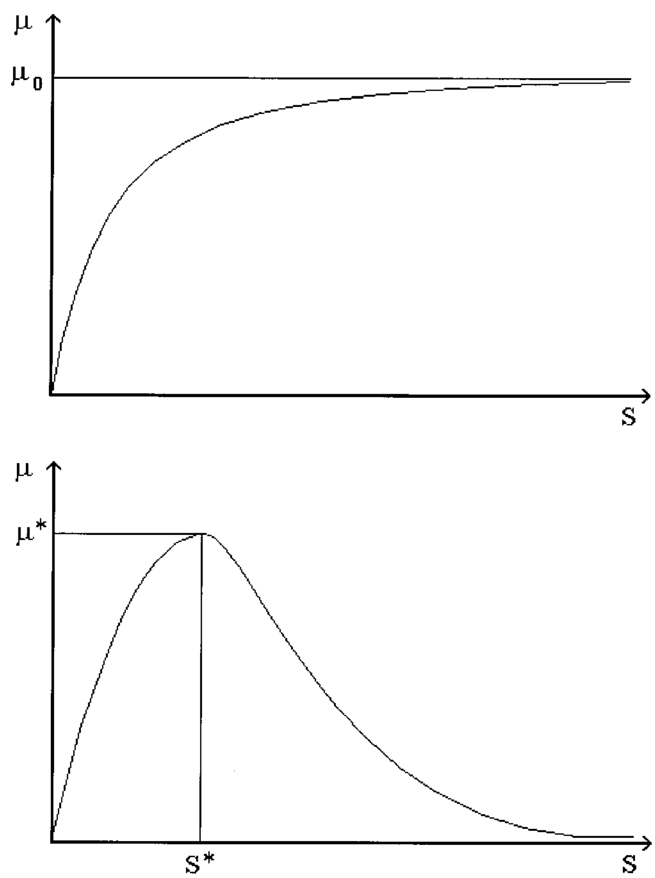

Figure 2. *Top*: Monotonic specific growth rate: Monod law. *Bottom*: Haldane law

increasing, i.e. $d\mu/dS > 0$ for every $S \geqslant 0$. If (H1) is satisfied then the time optimal problem for the system (11) will be uniquely solved by the feedback control law

$$F_{\text{in}} = \begin{cases} 0, & \text{if } V = V_{\text{f}}, \\ F_{\max}, & \text{if } V < V_{\text{f}}, \end{cases} \tag{20}$$

and the reaction will be finished if $(V = V_{\text{f}}) \wedge (S \leqslant S_{\min})$.

Proof. From (H1) it follows that there is no point of the set $\{S > \tilde{S}_{\text{in}}(V)\}$ in the attainable set $R(x_0) \cap R(\mathbf{X}_{\text{f}})$. Because $\mu(S)$ is strictly monotone increasing the sign of the function $\omega(\mathbf{x})$ (see (18)) is negative in all the attainable set (except possible on the right boundary $\phi(t, F_{\max}, \mathbf{x}_0)$). According to Green's theorem the global and unique time optimal trajectory consists at most of two arcs:

(i) First the arc $\phi(t, F_{\max}, \mathbf{x}_0)$ will be followed until $V = V_{\text{f}}$ is reached, and
(ii) if the substrate concentration is still bigger than required, i.e. $S > S_{\min}$, then a trajectory arc corresponding to $\phi(-t, 0, \mathbf{X}_{\text{f}})$ should be followed (backwards) until the desired set $\mathbf{X}_{\text{f}}$ has been reached.

The feedback control law for F_{in}, necessary to obtain this trajectory, can be expressed as in (20), and its uniqueness is assured by the fact that $\Delta(\mathbf{x}) \neq 0$ on the trajectory. □

Remark 12

In the present case the control function is of the Bang–Bang type, as is typical for time optimal control problems. The same solution applies for the original problem with system (7).

Remark 13

For the implementation of the feedback control law (20) it is necessary to measure the volume of the tank V, to determine the end of the fill phase, and the concentration of substrate S, to decide the end of the reaction phase, i.e. when $S_{\min}$ has been reached.

5.2. *Non-monotonic $\mu(S)$ with one maximum point (Haldane law)*

The prototype of this class is the Haldane law (see Figure 2), which is described by the equation

$$\mu(S) = \frac{\mu_0 S}{K_s + S + S^2/K_i} \tag{21}$$

where K_s (M L^{-3}) is the *affinity* constant, K_i (M L^{-3}) is the *inhibition* constant and μ_0 (T^{-1}) is the maximum specific growth rate. The maximum value of the specific growth rate μ^* for the substrate concentration S^* is characteristic for the Haldane law.

This type of specific growth rates are typical for processes where the substrate is a toxic substance and, for big concentrations, inhibits the activity of the biomass.[3,20] This is the case in the treatment of industrial wastewater.

The following theorem gives the solution of the time optimal control problem for a generic class of Haldane-type specific growth rates.

Theorem 14

Let $\mu(S)$ be positive (i.e. $\mu(S) > 0$ for $S > 0$), $\mu(0) = 0$, bounded (i.e. $\mu(S) \leqslant M$ for every $S > 0$ and for some positive constant M) and once continuously differentiable. Furthermore let $\mu(S)$ be a Haldane-type function, i.e. it is monotonically increasing ($\mathrm{d}\mu/\mathrm{d}S > 0$) up to the point S^*, where the maximum value μ^* is reached, and for $S > S^*$ the function is monotonically decreasing ($\mathrm{d}\mu/\mathrm{d}S < 0$). If (H1) is satisfied, $\tilde{S}_{\mathrm{in}}(V) \geqslant S^*$ for $V_0 \leqslant V \leqslant V_\mathrm{f}$, $S_{\min} \leqslant S^*$ and $F_{\sin} \leqslant F_{\max}$, then the time optimal control problem for the system (11) will be uniquely solved by the feedback control law:

$$F_{\mathrm{in}}^* = \begin{cases} \text{(1) If } V = V_\mathrm{f} \text{ then } F_{\mathrm{in}} = 0 \text{ until } S \leqslant S_{\min}, \text{ then stop} \\ \text{(2) If } V < V_\mathrm{f} \text{ and } S = S^* \text{ then } F_{\mathrm{in}} = F_{\sin} \text{ until } V = V_\mathrm{f}, \text{ then go to (1)} \\ \text{(3) If } V < V_\mathrm{f} \text{ and } S > S^* \text{ then } F_{\mathrm{in}} = 0 \text{ until } S = S^*, \text{ then go to (2)} \\ \text{(4) If } V < V_\mathrm{f} \text{ and } S < S^* \text{ then } F_{\mathrm{in}} = F_{\max} \text{ until } S = S^*, \text{ then go to (2)} \\ \quad\; \text{or until } V = V_\mathrm{f}, \text{ then go to (1)} \end{cases} \tag{22}$$

where $F_{\sin}$ is the control function that achieves that $S = S^*$, i.e.

$$F_{\sin} = \frac{\mu^* V X}{Y(\tilde{S}_{\mathrm{in}}(V) - S^*)} \tag{23}$$

Proof. From (H1) it follows that there is no point of the set $\{S > \tilde{S}_{\mathrm{in}}(V)\}$ in the attainable set $R(\mathbf{x}_0) \cap R(\mathbf{X}_\mathrm{f})$. Because $\mu(S)$ is monotonically increasing up to S^* and then monotonically decreasing, the function $\omega(\mathbf{x})$ (see (18)) is negative for $S < S^*$, zero for $S = S^*$, and positive for $S > S^*$ (except possible on the right boundary $\phi(t, F_{\max}, x_0)$), (see Figure 1). According to Green's theorem the global and unique time optimal trajectory consists of at most three arcs. They will be described depending on the position of the initial point $\mathbf{x}_0$:

1. If $V_0 = V_\mathrm{f}$: The trajectory $\phi(-t, 0, \mathbf{X}_\mathrm{f})$ will be followed (backwards) until the final point $S = S_{\min}$ will be reached.
2. If $(V_0 < V_\mathrm{f}) \wedge (S_0 > S^*)$: the optimal trajectory consists of three arcs: (see Figure 3)
   (a) Follow the trajectory arc $\phi(t, 0, \mathbf{x}_0)$ until $S = S^*$,
   (b) then follow the trajectory $\phi(t, F_{\mathrm{sing}}, [S^*, V_0])$, that maintains $S = S^*$, until the tank is filled $V = V_\mathrm{f}$. This is possible since $F_{\sin} \leqslant F_{\max}$.

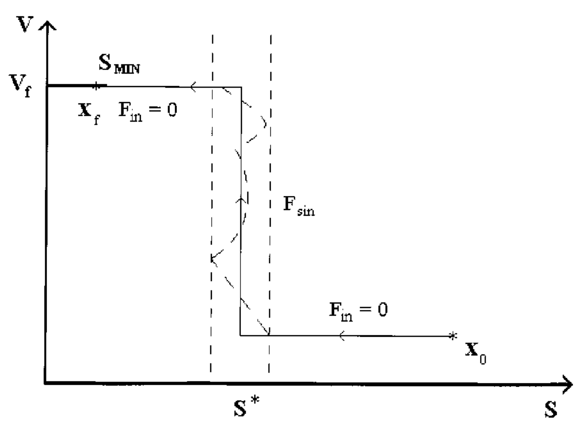

Figure 3. Time optimal trajectory for a Haldane-type function (—). Boundary layer and (possible) trajectory for the Robust feedback control law (– –)

(c) If the concentration of substrate is still bigger than required ($S > S_{min}$), the trajectory $\phi(t, 0, [S^*, V_f])$ will be followed until $S = S_{min}$.

3. If $(V_0 < V_f) \wedge (S_0 < S^*)$ the time optimal trajectory is: Follow $\phi(t, F_{max}, \mathbf{x}_0)$ until $S = S^*$ (in this case go to step (ii) (b)) or $V = V_f$ (then go to step (ii) (c)).

The feedback control low for F_{in}, necessary to obtain all this trajectories, can be expressed as in (22), its uniqueness is assured by the fact that $\Delta(\mathbf{x}) \neq 0$ on the trajectory and its admissibility is assured by the hypothesis $F_{sin} \leqslant F_{max}$.

F_{sin} is the control function that makes $S = S^*$, which is a *singular* arc of the trajectory From equation (7), making $dS/dt = 0$, it is easy to arrive to the expression (23) for F_{sin}. □

Remark 15

The control law (22) is not, in general, of Bang–Bang type, because it can have a singular arc. It can be implemented, for the original system (7) if all state variables X, S and V and the disturbance $\tilde{S}_{in}(V)$ or $S_{in}(t)$ can be measured.

6. ROBUST FEEDBACK CONTROL LAW

For the implantation of the optimal control law (20) or (22) it is necessary to measure all the state variables, to know exactly the plant parameters and, what is even worse, to measure the input substrate concentration. This is unrealistic and is unlikely to be found in practice. Furthermore, if the parameters of the plant are uncertain then the control law (22) can be far from optimality. In this section it will be shown that if the substrate concentration is measured, the final volume of the tank can be detected and only the critical substrate concentration S^* (for a Haldane-type law) is known, then a robust feedback control can be implemented such that its trajectories are arbitrarily near optimality, even if the input substrate concentration and most of the parameters are not known. For the case of Monod-type laws the control law (20) is already robust and it is only necessary to determine when V_f and S_{min} have been reached.

First of all note that the optimal feedback law for the non-monotonic case (22) can be implemented as

$$F_{in} = \begin{cases} 0 & \text{if } (V = V_f) \vee (S > S^*) \\ F_{sin} & \text{if } (S = S^*) \wedge (V < V_f) \\ F_{max} & \text{if } (S < S^*) \wedge (V < V_f) \end{cases} \tag{24}$$

It is easy to see that $S = S^*$ is a *sliding surface* and that the control law is discontinuous across it. Because of noise, disturbances and necessary imperfection of the implementation of the control this leads to *chattering*, what is highly undesirable in practice. It is also easy to note that the singular control (23) is just the *equivalent control* in Filippov's construction.[21] Using well-known techniques in the sliding mode control the discontinuous law can be smoothed by different means in such a way, that the trajectory stays arbitrarily near to the sliding surface. However it is not clear that the so obtained trajectory is also arbitrarily near optimality. It will be shown that any (smoothed) control law that maintains the trajectory in an ε-boundary layer is also ε-time optimal.

Theorem 16

Let the hypothesis of Theorem 14 be satisfied. Suppose that the optimal control law (22) is replaced by one of the form

$$F_{\text{in}}^{\varepsilon} = \begin{cases} 0 & \text{if } (S \geqslant S^* + \varepsilon) \vee (V = V_{\text{f}}) \\ F & \text{if } (S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon) \wedge (V < V_{\text{f}}) \\ F_{\max} & \text{if } (S \leqslant S^* - \varepsilon) \wedge (V < V_{\text{f}}) \end{cases} \tag{25}$$

where

$$0 < \varepsilon < \min\left(S^*, \frac{\rho(\mathbf{z}_0)}{YV_0} + \frac{W(V_0)}{V_0} - S^*, \frac{\rho(\mathbf{z}_0)}{YV_{\text{f}}} + \frac{W(V_{\text{f}})}{V_{\text{f}}} - S^* \right)$$

and F is any function that has values between 0 and $F_{\max}$ when the trajectory is within the boundary layer

$$B_{\varepsilon} = \{(X, S, V) | S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon\}$$

neighbouring the sliding surface. Then for every initial condition $\mathbf{x}_0 \in \Omega_{\text{A}} J[F_{\text{in}}^{\varepsilon}] = J[F_{\text{in}}^*] + T(\varepsilon)$, such that $\lim_{\varepsilon \to 0^+} T(\varepsilon) = 0$, and $T(\varepsilon)$ is bounded for every $\mathbf{x}_0$. In other words the time along the trajectory $\phi(t, F_{\text{in}}^{\varepsilon}, \mathbf{x}_0)$ can be made arbitrarily near to the optimal time by decreasing the width of the boundary layer B_{ε} (see Figure 3).

Proof. Fix $\varepsilon > 0$ and $\mathbf{x}_0$. Consider two cases: whether the optimal trajectory touches or does not touch the set $B_{\varepsilon}^0 \doteq B_{\varepsilon} \backslash \{S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon, V = V_{\text{f}}\}$. If it does not then $T(\varepsilon) = 0$, since then $\phi(t, F_{\text{in}}^{\varepsilon}, \mathbf{x}_0)$ and $\phi(t, F_{\text{in}}^*, \mathbf{x}_0)$ are identical.

In the other case it will be shown that if $\phi(t, F_{\text{in}}^*, \mathbf{x}_0)$ or $\phi(t, F_{\text{in}}^{\varepsilon}, \mathbf{x}_0)$ touches once B_{ε}^0, then it will stay in B_{ε}^0 and will converge to the set $\{S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon, V = V_{\text{f}}\}$ where it can eventually leave B_{ε}. For this it is enough to show that on the boundaries $\Gamma^+ = \{(X, S, V) | S = S^* + \varepsilon\}$ and $\Gamma^- = \{(X, S, V) | S = S^* - \varepsilon\}$ of B_{ε}^0 the vector field points into the interior of B_{ε}^0, when this intersection lies in the region given by $S < W(V)/V + \rho(\mathbf{z}_0)/(YV)$. For the points of the intersection that lie outside that region then by the hypothesis of the theorem and because of the results of Proposition 2 they cannot be reached and the trajectory cannot go out of B_{ε}^0 through such points. Consider first the vector field of system (11) on Γ^+, for F_{in}^* or $F_{\text{in}}^{\varepsilon}$, given by the vector

$$\mathbf{f}(\mathbf{x}) = \left[-\frac{1}{Y} \mu(S)(Y(W(V)/V - S) + \rho(\mathbf{z}_0)/V), 0 \right]^{\text{T}}.$$

$\mathbf{f}(\mathbf{x})$ points into the set B_{ε}^0 for every $V > 0$. Now on the other boundary Γ^- the vector field

$$\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})F_{\max} = \left[-\frac{1}{Y} \mu(S)(Y(W(V)/V - S) + \rho(\mathbf{z}_0)/V) + \frac{\tilde{S}_{\text{in}}(V) - S}{V} F_{\max}, F_{\max} \right]^{\text{T}},$$

for either F_{in}^* or $F_{\text{in}}^{\varepsilon}$, also points into B_{ε}^0 for every $0 < V < V_{\text{f}}$. This follows from the fact that for every $0 \leqslant S < S^*$, and $V > 0$ the first component of $\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})F_{\max}$,

$$\gamma(S, V) = -\frac{1}{Y} \mu(S)(Y(W(V)/V - S) + \rho(\mathbf{z}_0)/V) + \frac{\tilde{S}_{\text{in}}(V) - S}{V} F_{\max},$$

is strictly positive ($\gamma(S, V) > 0$), if the hypothesis $F_{\text{sin}} \leqslant F_{\max}$ is satisfied and $\mu(S)$ is a Haldane-type function. To see why note first that for $V > 0$, $\gamma(0, V) > 0$, and $F_{\text{sin}} \leqslant F_{\max}$ implies that for $V > 0$,

$\gamma(S^*, V) > 0$. These two conditions cannot be simultaneously satisfied if $\gamma(S, V) = 0$ has a solution for $S \in (0, S^*)$. This follows easily by writing the equation $\gamma(S, V) = 0$ as

$$\mu(S) + \frac{S - \tilde{S}_{\text{in}}(V)}{V(Y(W(V)/V - S) + \rho(\mathbf{z}_0)/V)}\, Y F_{\max} = 0$$

and noting that both terms of this equation are monotonically increasing functions of S for $S \in (0, S^*)$.

Now it will be shown that if a trajectory starts in B_ε^0 it will reach the set $\{S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon, V = V_{\text{f}}\}$, where it can eventually leave B_ε. For this note that for a point in the boundary layer $S^* - \varepsilon \leqslant S \leqslant S^* + \varepsilon$, and therefore $\mu_\varepsilon \leqslant \mu(S) \leqslant \mu^*$, where $\mu_\varepsilon \doteq \min[\mu(S^* + \varepsilon), \mu(S^* - \varepsilon)]$. From (7), i.e. $\dot{\gamma} = \mu(S)\gamma$, where $\gamma \doteq XV$, and standard differential inequalities it follows easily that for every trajectory starting in $t = 0$ in B_ε^0 at $X(0) = X_0$, $V(0) = V_0$, i.e. $\gamma_0 = X_0 V_0$, for any time $t \geqslant 0$ the inequality $\gamma_0 \exp(\mu_\varepsilon t) \leqslant \gamma(t) \leqslant \gamma_0 \exp(\mu^* t)$ is satisfied. Since (11) $\gamma = Y(W(V) - SV) + \rho(\mathbf{z}_0)$ and using the conditions on ε it is easy to see that the maximal ($T_{\max}^\varepsilon$) and minimal ($T_{\min}^\varepsilon$) times of permanence of a trajectory in the set B_ε are given by

$$T_{\max}^\varepsilon = \frac{1}{\mu_\varepsilon} \ln\left(\frac{\gamma_{\text{f}}^* + Y V_{\text{f}} \varepsilon}{\gamma_0^* - Y V_0 \varepsilon}\right) \quad \text{and} \quad T_{\min}^\varepsilon = \frac{1}{\mu^*} \ln\left(\frac{\gamma_{\text{f}}^* - Y V_{\text{f}} \varepsilon}{\gamma_0^* + Y V_0 \varepsilon}\right),$$

where $\gamma_0^* = Y(W(V_0) - S^* V_0) + \rho(\mathbf{z}_0)$ and $\gamma_{\text{f}}^* = Y(W(V_{\text{f}}) - S^* V_{\text{f}}) + \rho(\mathbf{z}_0)$. Since the time difference between the two trajectories obtained by the two controls F_{in}^* and $F_{\text{in}}^\varepsilon$ is only caused by the time difference in the set B_ε, i.e. $T^\varepsilon - T_{\text{opt}}^\varepsilon$, where T^ε is the residence time in B_ε with the input $F_{\text{in}}^\varepsilon$ and $T_{\text{opt}}^\varepsilon$ is the residence time in B_ε with the input F_{in}^*. It is clear that $T_{\min}^\varepsilon \leqslant T_{\text{opt}}^\varepsilon \leqslant T^\varepsilon \leqslant T_{\max}^\varepsilon$ and that for every $\mathbf{x}_0$ considered $T_{\max}^\varepsilon$ is bounded and therefore $T(\varepsilon)$ is bounded. Furthermore since $\mu(S)$ is continuous, bounded away from 0 in B_ε and $\lim_{\varepsilon \to 0} \mu_\varepsilon = \mu^*$ it follows that $\lim_{\varepsilon \to 0^+} T^\varepsilon = \lim_{\varepsilon \to 0^+} T_{\text{opt}}^\varepsilon = (1/\mu^*) \ln(\gamma_{\text{f}}^*/\gamma_0^*)$ and therefore $\lim_{\varepsilon \to 0^+} T(\varepsilon) = 0$. □

For the implantation of this robust control law it is only necessary to know: that the specific growth rate is a Haldane-type law (the specific form is not important); the value of S^*, the measurement of S, the moment when $V = V_{\text{f}}$, and that the conditions of the theorem are satisfied. It is therefore robust against all parameters of the plant (except for $S^* = \sqrt{K_s K_I}$), the value of S_{in}, the value of the biomass concentration X, and the exactness in the measurement of V, since only an on–off controller in this variable is necessary. It is clear from the foregoing theorem that $T(\varepsilon)$ is small if ε is small and if $(\mu^* - \mu_\varepsilon)$ is also small. On the other side if ε is small the control input is more likely to chatter and the frequency band of the input is higher, what is not desirable. Moreover if the disturbance S_{in} changes a lot the control input has to switch more frequently. Therefore there is a trade-off between been near to optimality, the frequency band of the control signal and the uncertainty in the parameters (to determine an upper bound for $(\mu^* - \mu_\varepsilon)$) and in the disturbance. Finally a possible and simple form of F in $F_{\text{in}}^\varepsilon$ is $F = (1 - (S - S^*)/\varepsilon) F_{\max}/2$, a linear function in B_ε.

7. EXAMPLE OF APPLICATION TO AN INDUSTRIAL WASTEWATER TREATMENT PLANT

Often in practice the control strategy of a SBR for the industrial wastewater treatment is very simple: The tank will be filled as fast as possible and the complete cycle of the SBR is fixed to be 24 h. In this case information about the state of the process is not used for its control. The results of this paper can be used to implement a different control strategy for the SBRs. To illustrate the advantages of using the *optimal-strategy* some simulations for a realistic plant will be run for the optimal control and for a *batch-strategy*, for which the reactor will be filled as fast as possible and the reaction phase will be stopped as soon as $S \leqslant S_{\min}$.

The parameters of the model have been taken from Reference 20. The substrate to be degraded is phenol. Because of the inhibitory effect of phenol on the biomass, the specific growth rate follows the Haldane law (21).

The values of the used parameters were: $V_f = 50\ \mathrm{m}^3$, $F_{\max} = 50\ \mathrm{m}^3\,\mathrm{h}^{-1}$, $K_s = 2\ \mathrm{mg\,l}^{-1}$, $K_i = 50\ \mathrm{mg\,l}^{-1}$, $\mu_0 = 0{\cdot}072\ \mathrm{h}^{-1}$ and $Y = 1/2$. The substrate concentration in the input flow S_{in} will be considered to be $200\ \mathrm{mg\,l}^{-1}$ until the reactor has reached a volume of $25\ \mathrm{m}^3$ and there it changes abruptly to $S_{\mathrm{in}} = 400\ \mathrm{mg\,l}^{-1}$ until the end (this function is not continuously differentiable but can be approximated by one with any desired degree of accuracy).

As initial condition (X_0, S_0, V_0) for the first cycle and final condition $(S_{\min}, V_f)$ for every cycle the values: $X_0 = 13\,000\ \mathrm{mg\,l}^{-1}$, $S_0 = 50\ \mathrm{mg\,l}^{-1}$, $V_0 = 5\ \mathrm{m}^3$, $S_{\min} = 1\ \mathrm{mg\,l}^{-1}$ and $V_f = V_{\max}$ were used. As initial values of X and S for the second and following cycles will be considered the final values of the foregoing cycle. In each cycle a total time of 0·65 h has been included for the settling and drawing phases.

Figure 4 show the simulations results for several SBR-cycles using both strategies. A robust implantation was used with $\varepsilon = 0{\cdot}05$. In them the time behaviour of two relevant variables is shown: S, the concentration of phenol in the tank ($\mathrm{mg\,l}^{-1}$) and F_{in}, the input water flow to the tank ($\mathrm{m}^3\,\mathrm{h}^{-1}$). Note that the amount of phenol treated in each cycle is equal for both strategies.

Note first that while one cycle is completed with the batch-strategy almost two cycles have been done by the optimal-strategy. This means that the optimal control law allows to treat almost two times more water than with the batch-strategy. If, as usual in practice, a 24 h-strategy is implanted instead of the batch-strategy the comparison with the optimal-strategy is obviously worse. If the optimal control can be implanted a much smaller reactor can treat the same amount of water than the one needed by the other control methods.

From Figure 4 one can also notice that the substrate concentration in the reactor with the batch-strategy is much higher than with the optimal one. Since the substrate is a toxic substance these high concentrations can cause the death of the biomass, an effect that has not been included in the model (1), but that can be observed experimentally, and makes the optimal-strategy also more attractive for the operation of the treatment plant. Moreover the substrate concentration in the tank is independently of the concentration in the input flow (S_{in}) for the optimal-strategy whereas for the batch-strategy an increase in S_{in} causes an increase in S in the tank (this is called a Shock Load) and reduces the performance of the plant. This implies that the optimal-strategy is an excellent solution for Shock-Loads. The predicted robustness of the algorithm was tested by simulations (not shown).

There is obviously an advantage in using the optimal strategy or some feedback strategy instead of the batch-strategy or the usual one of 24 h per cycle. The complexity in the measurement of the state variables and in the equipment to implant the feedback control law is the pay off for the better performance of the plant. This is really a challenge because the difficulty in the on line measurement of the substrate concentration S and of the biomass concentration X.

8. CONCLUSIONS

Motivated by the problem of efficiency optimization of an SBR used in the wastewater treatment, the time optimal control problem of a family of models of such reactors has been solved. An important difference with existing works is the consideration of a variant substrate concentration in the input flow, which is the main disturbance for these processes. For two different general

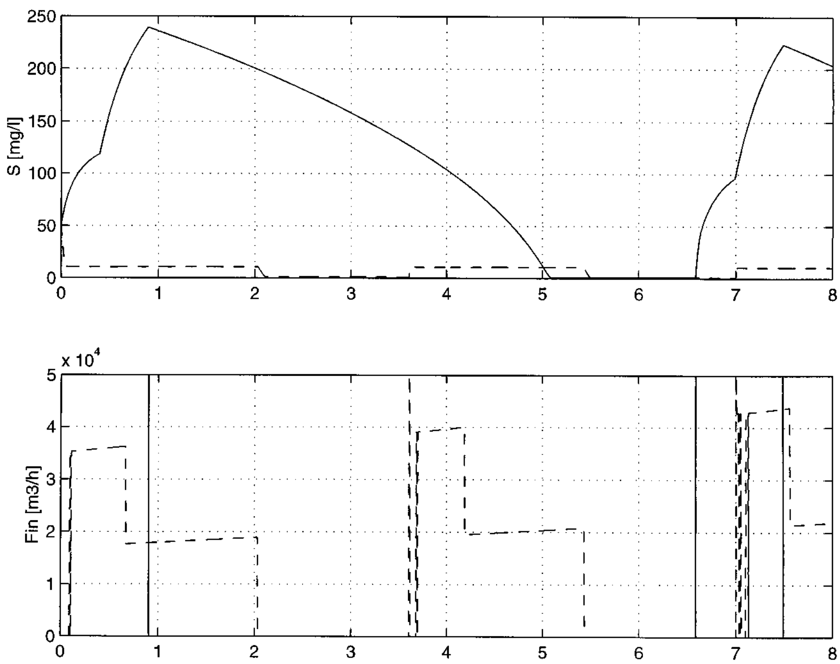

Figure 4. Simulation of some cycles of the SBR using the batch (—) and the optimal (– –) strategies. *Top*: Substrate concentration, *Bottom*: Input flow

forms of the specific growth rate $\mu(S)$, which are often found in practice, the solution of the optimal problem has different characteristics. If $\mu(S)$ is a Monod-type function the solution is of Bang–Bang type, while it has a singular arc if the specific growth rate is a Haldane-type function.

The solution method for the time optimal problem was, instead of the usual Maximum Principle of Pontryagin, a method based on Green's theorem. Global and necessary and sufficient conditions for optimality were obtained and the solution of the singular case was possible using this technique. As the original model is of third order and the method is only usable for systems in the plane, an equivalent second-order description of the original model had to be found. This was possible because the uncontrollability of that model, so that a minimal description of it is of second order, and therefore suited for Green's method. Analytical instead of numerical solutions for the problem were obtained. This has lead to the development of a robust feedback control law that is, on the one side, as near to optimality as desired and, on the other side, has important robustness properties. Furthermore for the implementation of this control law it is necessary neither to measure all the state variables nor the perturbation signal, and only one parameter is really necessary to be known. There is of course a trade off between optimality and robustness.

Simulations of a realistic model of an industrial wastewater treatment plant have shown the advantages of using an optimal strategy in the control of the plant. The increase in efficiency is high, what reduces the costs of operation and the size of the plant. Furthermore the solution of the usual problem of shock-loads for batch and continuous reactors, and the death of the microorganisms caused by them is another positive aspect of the optimal-strategy.

ACKNOWLEDGEMENT

Work supported by DGAPA, UNAM, Mexico under Project PAPIIT IN118098.

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