# Practical Optimal Control of Fed-Batch Bioreactors for the Waste Water Treatment

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#### Abstract

Optimal operation of fed-batch bioreactors is an important practical issue. Since control actions are saturation-limited, the optimal control consists usually of both singular and bangbang arcs. However, its realization requires good model knowledge and also the measurement of all state variables, requirements rarely satisfied in real applications. In this paper a method is proposed, for a class of bioreactors, to robustly optimize the operation when few measured variables are available and the model is uncertain. Such control law is justified and its properties analyzed. The case of a bioreactor for treating toxicants in a Waste Water Treatment Plant is thoroughly studied, and experimental results in a lab-scale bioreactor are presented. The method can be applied also for other applications, as in biotechnology.

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# 1 Introduction

Activated sludge is an aerobic biological process in which waste water 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 waste waters 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. They offer, for example, greater flexibility in control strategy, but 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.

With the beginning of the fill phase, or some time later, the aerator is turned on. The reaction (or aeration) phase which now begins should last until the biodegradable portion of the organic waste water 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.

Many other important industrial fermentation processes, as for the production of antibiotics and enzymes, are carried out using bioreactors operated in fed-batch mode. Since it is reasonable to improve their performance, optimal control theory has been used to determine the best control policy [11, 8, 7]. Such strategy can be described as a feedback control law, and it is usually necessary to know perfectly the model of the plant, and to measure the whole state to implement it. In many applications these two conditions are very restrictive: a perfect model and parameter knowledge is very often unrealistic, and in biotechnology and waste water treatment it is either impossible or very expensive to measure all state variables. In order to cope with the first problem different robust approaches have been proposed in the literature. Most often different adaptive algorithms identify the parameters of the (otherwise assumed well known) mathematical model, and adapt accordingly the control strategy [1, 14, 13]. Adaptive Extremum-Seeking strategies have been also proposed [6, 12]. Although the methodology is most appropriate for continuous reactors, where an optimal steady state operation is searched, under suitable conditions it can also operate correctly for fed-batch processes [3].

In this work a different approach to deal with the lack of measurements and the uncertainty in the model, while optimizing operation, of a class of bioreactors will be proposed. The main idea is based on the following observations. Usually, the exact optimal control, when the realistic assumption of limited input variables is done, can be decomposed in bang-bang and singular arcs. When this solution can be implemented via feedback the information required for the bang-bang part is very low, and its implementation is very robust to model uncertainties. More problematic is the determination and implementation of the singular arc. It requires basically a good knowledge of the model and parameters of the plant, and it is usually very sensitive to uncertainties. Our method proposes to replace the sensitive and smooth singular control by a bang-bang one that maintains the system trajectory around the singular surface. The optimality loss can (theoretically) be made as small as desired [4, 7]. The advantage of this replacement is that it is usually very robust against uncertainties and, for its implantation, a reduced quantity of information is required [7]. The robustness of this implementation is linked to the well-known properties of Sliding Mode Control [5, 10]. The requirement of low quantity of information is related to the fact that it is only necessary to determine the singular surface in the state space. This surface is usually associated to some events on internal variables. If such events could be software-sensed using just the measurable variables, then a practical solution is feasible. Moreover, if the switching or singular surfaces are robustly related to these variables, the approach can be made robust against model changes or uncertainties.

In the following section the class of problems for which these ideas are developed will be introduced. In Section 3 the previously outlined strategy will be carried out for these problems. In Section 4 some experimental results will be presented.

## 2 Model description and problem formulation

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

$$\dot{X}(t) = \left(\mu(S(t)) - \frac{F_{in}(t)}{V(t)}\right) X(t) ,$$
  
$$\dot{S}(t) = -\frac{1}{Y_{X/S}} \mu(S(t)) X(t) + \frac{F_{in}(t)}{V(t)} \left(S_{in}(t) - S(t)\right) , \qquad (1)$$
  
$$\dot{V}(t) = F_{in}(t) ;$$

where:

X	:	Biomass concentration in the reactor, $[ML^{-3}]$		
S	:	Substrate concentration in the reactor, $[ML^{-3}]$		
V	:	Volume of water in the tank, $[L^3]$		
$\mu(S)$	:	Specific growth rate, $[T^{-1}]$		
$F_{in}$	:	Influent water flow to the reactor, $[L^3T^{-1}]$		
$S_{in}$	:	Substrate concentration in the input flow, $[ML^{-3}]$		
$Y_{X/S}$	:	Biomass/Substrate yield coefficient.		

 $F_{in}$ , the control variable, can only take values in a positive and closed interval  $F_{in} \in [0, F_{max}]$ ,  $F_{max} > 0$ , and all three state variables (X, S, V) have to be positive, i.e.  $X \ge 0$ ,  $S \ge 0$  and  $V \ge 0$ . 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. For any system variable  $\phi$  let us denote its value at instant t as  $\phi(t, t_0, \mathbf{z}_0, F)$  for input F, being  $\mathbf{z}_0$  the state at  $t_0 \le t$ . It will be also assumed that  $Y_{X/S}$  is constant and that  $\mu(S)$ is defined for  $S \ge 0$ ,  $\mu(0) = 0$ , is positive (i.e.  $\mu(S) > 0$  for S > 0), bounded (i.e.  $\mu(S) \le M$  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 such that  $S_{in}(t) \ge 0$ .

The objective of such a bioreactor in a Waste Water Treatment Plant (WWTP) is to bring the concentration of the substrate in the tank S below a specified level  $S_{\min}$ , while the volume is brought from  $V_0$  to  $V_f$ , where  $0 < V_0 < V_f \leq V_{max}$ . Usually in practice the concentration of pollutants in the water to be treated is not uniformly distributed, what is reflected in the fact that  $S_{in}(t)$  in model (1) is not constant. For waste water treatment processes this is in fact one of the main disturbances. We want to deal with the following physically meaningful situation: Consider that the waste water to be treated is fed to the reactor, and that its pollutant concentration  $S_{in}$  is unknown and can

change arbitrarily. It is of course of interest to optimize the efficiency of the process, defined as the quantity of pollutant treated per unit of time. Since the process is cyclic one has to maximize the efficiency per cycle  $\epsilon_c$ , given by

$$\epsilon_c = \frac{C}{T_c},$$

i.e. the quantity of substrate degraded during the cycle C divided by  $T_c$ , the cycle time, where the value of  $T_c$  depends on the input function  $F_{in}(t)$ . Since under realistic situations the amount of pollutant to be treated in the reactor C does not depend on the form it is fed, i.e. it is a constant independent of  $F_{in}$ , the maximization of  $\epsilon_c$  coincides with the minimization of the cycle time  $T_c$  [7]. 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. The cost functional to be minimized is therefore the reaction time  $T_r$ , i. e.  $J[F_{in}] = \int_0^{T_r} d\tau$ . Therefore the problem is to find an time optimal control law for the input variable  $F_{in}$ . This is one that brings the system from a given initial state  $\mathbf{z}_0 = [X_0, S_0, V_0]$  to a final one  $\mathbf{z}_f = [X_f, S_f, V_f]$ , in a set of desired final states  $\mathbf{Z}_f \doteq \{\mathbf{z}_f \mid 0 \leq S_f \leq S_{\min}, V_f\}$ , 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

$$0 \le F_{in} \le F_{\max} , \qquad (2)$$

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

$$\Omega \doteq \{ (X, S, V) \mid 0 < X_{\min} \le X \le X_{\max} , \ 0 \le S \le S_{\max} , \ 0 < V_{\min} \le V \le V_{\max} \} , \qquad (3)$$

where  $S_{\max}$  is a physically meaningful upper limit for S. Note that if  $X_0 > 0$  then X(t) > 0 for



Figure 1: Inhibitory-type biomass specific growth rate. The dotted line depicts a measurable  $\gamma = (a\mu + b) c$ .

every input of the system (1). The restrictions for the volume V come from the fact that the tank cannot be completely emptied and that it has finite physical dimensions.

Depending on the nature of the pollutants the specific growth rate  $\mu(S)$  may adopt one of two typical forms. When the substrate does not inhibit the activity of the biomass,  $\mu(S)$  is monotonic, i.e. it is characterized by the fact that  $\frac{d\mu}{dS} > 0$  for every  $S \ge 0$ . A typical expression is the Monod law given by

$$\mu\left(S\right) = \frac{\mu_0 S}{K_s + S} , \qquad (4)$$

where  $K_s \ [ML^{-3}]$  is the Monod constant and  $\mu_0 \ [T^{-1}]$  the maximum specific growth rate. For the treatment of toxic substances, encountered for example in industrial waste waters, even for relatively low substrate concentrations the activity of the biomass may be inhibited [9].  $\mu(S)$  is in this case non-monotonic (see Figure 1), i.e. it is monotonically increasing  $(\frac{d\mu}{dS} > 0)$  up to the point  $S^*$ , where  $\mu(S)$  reaches its maximum value  $\mu^*$ , and for  $S > S^*$  the function is monotonically decreasing  $(\frac{d\mu}{dS} < 0)$ . The prototype of this class is the Haldane law, which is described by the equation

$$\mu(S) = \frac{\mu_0 S}{K_s + S + \frac{S^2}{K_T}} \quad , \tag{5}$$

where  $K_s \ [ML^{-3}]$  is the Affinity constant,  $K_I \ [ML^{-3}]$  is the Inhibition constant and  $\mu_0 \ [T^{-1}]$ is the specific growth rate coefficient. The maximum value of the specific growth rate  $\mu^*$  for the substrate concentration  $S^*$  is characteristic for the inhibitory-type laws (see Figure 1). Because of the complexity of the biochemical reactions involved, the functional description of the specific growth rate is usually not well known, and the functions (4) or (5) represent only approximations. For both kinds of specific growth rates the time optimal control strategy was found in [7]. However, the implementation of such a control law requires, in principle, the measurement of the state variables and a good knowledge of the model.

One of the main limitations in biotechnological processes, and particularly in WWTPs, is the availability of on-line measurements. In general, it is difficult and expensive to measure biomass and substrate concentrations, but it is easy to measure volume, gaseous products and dissolved oxygen concentrations. For the aerobic WWTP described by (1) it will be assumed that only the volume level V, and the Dissolved Oxygen Concentration O are measured, whose dynamics is given by

$$\dot{O}(t) = -\left(\frac{1}{Y_{X/O}}\mu(S(t)) + b\right)X(t) + k_L a(O_s - O(t)) + \frac{F_{in}(t)}{V(t)}(O_{in} - O(t)) , \qquad (6)$$

where:

*O* has to be positive, i.e.  $O \ge 0$ . It will be also assumed that  $Y_{X/O}$ , b,  $O_{in}$ ,  $O_s$ , and  $k_L a$  are known constants. Note that the DO is affected by the system dynamics (1), but that this system is not influenced by the variations in the Oxygen concentration O. This approximation is valid when the DO is not a limiting reactant in the degradation reaction. For this process this condition has to be satisfied, since the behavior of the reactor undergoes a big change when anoxic or anaerobic conditions prevail in the reactor. This condition can be assured by a properly operating aeration system, that maintains the DO concentration above a minimal value, typically set to  $O_{\min} = 2 \text{ mg/l}$ . This one-sided coupling of the DO dynamics means that the DO is only used for measurement purposes, and leads to the independence of the time optimal control problem from the dynamics of O, i.e. it depends only on the state variables of (1).

The objective of this work is then to design a suboptimal time optimal control law that uses the measurable variables (V, O) and that is robust against uncertain specific growth rate model and uncertain parameters.

For monotone specific growth rates as (4) the time optimal control [7] is very simple: fill with  $F_{in} = F_{max}$  until the the reactor is full, i.e.  $V = V_f$ , and then switch to  $F_{in} = 0$  until the degradation is completed, i.e.  $S = S_{min}$ . In this case the implementation of the optimal control strategy requires neither measurements of state variables nor knowledge of system parameters, except that the specific

growth rate is monotone, and a mean to detect the end of the reaction phase is provided. For this reason, and to simplify the presentation, only the case of non-monotone specific growth rates as (5) will be considered. Note that for the plant (1), when the control variable attains its minimum value  $F_{in} = 0$ , then the substrate concentration decreases, since  $\dot{S} < 0$ . When the control variable attains its maximum value  $F_{in} = F_{max}$ , however, it is not always true that  $\dot{S} > 0$ . It will be assumed that **Assumption 1** For a given a constant value  $\hat{S} > 0$ , when the maximum input flow is applied,  $F_{in}(t) = F_{max}$ , the substrate concentration in the reactor increases, i.e.

$$\frac{dS}{dt}\Big|_{F_{in}=F_{\max}} = -\frac{1}{Y_{X/S}}\mu(S(t))X(t) + \frac{F_{\max}}{V(t)}\left(S_{in}(t) - S(t)\right) > \varepsilon , \qquad (7)$$

for every  $S(t) \leq \hat{S}$ , and every V and X in the region  $\Omega$ , and for some  $\varepsilon > 0$ .

Note that if in Assumption 1  $\hat{S} \leq S^*$ , then no inhibitory effect of the substrate appears caused by the filling, and the behavior of the reactor corresponds to one with monotonic specific growth rate. In the next section only the case  $\hat{S} \geq S^*$  will be analysed. From (7) it follows that  $S_{in} > \hat{S}$ has to be satisfied, and that  $\hat{S}$  will be reached in finite time, except when  $V = V_f$  is reached before. Since the first term in (7) is negative, i.e. it is the substrate degradation rate, the injection rate of substrate, i.e. the second term in (7), has to be strong enough to compensate the first one.

## **3** Control Strategy

In this section the design of a control law that satisfies the imposed requirements will be explained in three steps. First the exact time optimal control (TOC) will be presented. It can be only implemented if the model is perfectly known and all state variables are available for measurement. In a second step two control strategies are described, to approximate the time optimal solution arbitrarily well. They are robust against model uncertainties of the plant, and only require the measurement of the substrate concentration S, in the first case, or a monotonic function of the the specific growth rate  $f(\mu)$ , in the second one. Since these controllers are based on the detection of some Events in the process, they will be named Event-Driven TOC (ED-TOC).

However, since neither S nor a function  $f(\mu)$  are available for measurement, these control strategies cannot be directly realized. Nevertheless using the variables measured on-line, i.e. volume V and DO concentration O, its time derivative  $\dot{O}$ , the control variable  $F_{in}$  and the knowledge of the parameters  $k_L a$ ,  $O_s$  and  $O_{in}$ , that can be easily estimated off or on-line, the signal

$$\eta(t) = k_L a V(t) (O_s - O(t)) + F_{in}(t) (O_{in} - O(t)) - V(t) \dot{O}(t)$$
(8)

can be calculated. From (6) it is easy to see that this signal corresponds to an output function of the system (1) given by

$$\eta = h\left(X, S, V\right) \triangleq \left(\frac{1}{Y_{X/O}}\mu\left(S\right) + b\right)B , \qquad (9)$$

where B(t) = V(t) X(t) is the total biomass in the reactor. If B would be a constant, then h(X, S, V) would serve as the function  $f(\mu)$  introduced before, and an approximate and robust ED-TOC could be implemented based on the measurement of  $\eta(t)$ . Although for bioreactors in the WWTP the total biomass B changes very little during a degradation cycle, and the conditions for the ED-TOC are practically satisfied, it is also true that B changes in time. For this reason in a third step the realization of the ED-TOC control law that uses the available measurement  $\eta(t)$ , and its suboptimal operation and robustness are studied.

Because of the dynamics of the DO in the process, it is possible to filter the noisy signal O and its derivative can be well approximated using differentiation algorithms for its use in (8). Finally, note that it is not necessary to know the values of  $Y_{X/O}$ , b and B in (9) to estimate  $\eta(t)$  from (8).

## 3.1 Exact Time Optimal Control (TOC) law

The following result from [7] gives the feedback law that solves the time optimal control problem for a generic class of Inhibitory-type specific growth rates, when the whole state is available.

**Theorem 2** [7] Let  $\mu(S)$  be positive (i.e.  $\mu(S) > 0$  for S > 0),  $\mu(0) = 0$ , bounded (i.e.  $\mu(S) \leq M$ for every S > 0 and for some positive constant M) and once continuously differentiable. Furthermore, let  $\mu(S)$  be a Inhibitory-type function, i.e. it is monotonically increasing  $(\frac{d\mu}{dS} > 0)$  up to the point  $S^*$ , where the maximum value  $\mu^*$  is reached, and for  $S > S^*$  the function is monotonically decreasing  $(\frac{d\mu}{dS} < 0)$ . If Assumption 1 is satisfied with  $\hat{S} > S^*$  for  $V_0 \leq V \leq V_f$ ,  $S_{in} > S^*$  and  $F_{sin} \leq F_{max}$ , then the time optimal control problem for the system (1) will be uniquely solved by the feedback control law:

$$F_{opt} = \begin{cases} 0 & if \quad V \ge V_f \text{ or } S > S^* \\ F_{sin} & if \quad S = S^* \\ F_{max} & if \quad S < S^* \end{cases}$$
(10)

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

$$F_{sin}(t) = \frac{\mu^* V(t) X(t)}{Y_{X/S}(S_{in}(t) - S^*)} \quad .$$
(11)

When  $V \ge V_f$  and  $S \le S_{\min}$  the reaction phase is finished.

This control law has (generically) three arcs: a first bang arc to bring the substrate concentration S to  $S^*$ , then a singular arc to maintain this substrate concentration until the reactor is full, and a third bang arc to degrade the rest of the substrate. The reaction phase finishes when  $V = V_f$  and  $S \leq S_{\min}$ , where  $S_{\min}$  is some (small) rest substrate value. The information required to implement the bang arcs is low: it is only necessary to know the value of  $S^*$ , and if  $S > S^*$  or if  $S < S^*$ .

However, the implementation of the singular arc requires much more knowledge on the model and measuring the internal variables: the (exact) values of  $Y_{X/S}$ ,  $S^*$ ,  $\mu^*$ , the measurement of the state variables S, V, X, and the measurement of the substrate concentration in the input flow  $S_{in}(t)$ . This is rarely satisfied in practice.

Let the function  $T(F, z_0)$  represent the time necessary to bring the initial state  $z_0$  to the target set  $Z_f = \{(X, S, V) \mid S \leq S_{\min} \land V \geq V_f\}$  using F as input (the other model parameters are fixed).  $T_{\text{opt}}(z_0) = T(F_{\text{opt}}, z_0)$  corresponds to the optimal path, i.e.  $T_{\text{opt}}(z_0) \leq T(F, z_0)$  for every admissible F. Note that in the state space  $\Omega$  the surfaces defined by  $S = S^*$  and  $V = V_f$  are, respectively, a singular and a switching surface.

## 3.2 Approximated optimal control law

Theorem 20.2 in [4] states that any trajectory of a nonlinear system can be arbitrarily well approximated by another one generated using a bang-bang control law. So, it is possible to approximate the time optimal trajectory generated by the control law (10) with a bang-bang one. That corresponds in this case to the approximation of the trajectory along the singular arc with a bang-bang one [7]. Since the performance criterion does not depend on the input function, and it is continuous with respect to the trajectories, then the optimal index is arbitrarily nearly reached by the approximated trajectory. For the problem at hand this has also been directly demonstrated by [7].

Approximate control laws can be generated in different forms. They differ basically in the information required to implement them. Some examples will be discussed in the following paragraphs.

#### **3.2.1** Suboptimal control law using S

If S is measurable and  $S^*$  is known, selecting values  $0 < S_l < S^* < S_h$  (see Figure 1) allow implementing the following bang-bang control law [7]

$$F_{\rm app} = \begin{cases} 0 & \text{if } V \ge V_{\rm max} \text{ or } S \ge S_h \\ F_{\rm max} & \text{if } S \le S_l \end{cases}$$
(12)

When  $S \leq S_{\min}$  and  $V \geq V_f$  the reaction phase is finished and the next phase (settling) may be started.

Note that if Assumption 1 is satisfied with  $\hat{S} > S_h$ , then when  $F_{in} = F_{max}$  the substrate concentration S grows until  $S = S_h$ . There the control is switched to  $F_{in} = 0$ , so that, since

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}}\mu(S)X < 0 , \ \forall \mathbf{z} \in \Omega \setminus \{S=0\} ,$$
(13)

S decreases until  $S = S_l$ , when the control is again switched to  $F_{in} = F_{max}$ . Therefore, whatever the initial condition the system trajectory tends to the set  $S_l \leq S \leq S_h$ , stays there until the reactor gets full, and then reaches the final set  $Z_f$ , finishing the reaction phase. It is important to note that the trajectory is confined to the set  $S_l \leq S \leq S_h$ , independently of and without knowledge of the parameters and/or the exact form of the growth rate and of the value of the input substrate concentration  $S_{in}$ . Making  $S_h - S_l$  sufficiently small the optimal trajectory can be approximated arbitrarily well.

**Theorem 3** [7] Suppose that system 1 is given, that Assumption 1 is satisfied with  $\hat{S} > S_h$ , that S is measured and that  $S^*$  is known. Then replacing the optimal control law  $F_{opt}$  of (10) by the approximate control law  $F_{app}$  of (12) the time to reach the target, from any initial condition  $\mathbf{z}_0 \in \Omega$ ,

$$T\left(F_{app}, S_l, S_h, z_0\right) = T_{opt}\left(z_0\right) + \Delta\left(S_l, S_h\right) ,$$

with  $\Delta(S_l, S_h)$  continuous and finite and  $\Delta \to 0$  as  $S_h, S_l \to S^*$ . This means that the target will be reached in finite time, and the time along the approximate trajectory can be made as near to the optimal one as desired. This is true for any form of the growth rate (positive if S positive), for unknown  $S_{in}$  and for any positive value of the parameter  $Y_{X/S}$ .

**Proof.** This is Theorem 16 in [7]. A sketch is given here for completeness, but for details see [7]. It is easy to see that the time spent by the portions of the optimal and of the approximate trajectories when S is outside the set  $S_l \leq S \leq S_h$  is the same, and so  $\Delta(S_l, S_h)$  corresponds to the increased time the approximate trajectory spends in  $S_l \leq S \leq S_h$ . Define  $\bar{\mu} = \min(\mu(S_l), \mu(S_h)) \leq \mu^*$  as the minimal value the specific growth rate can have while the trajectory is in the interval  $S_l \leq S \leq S_h$ . Since  $\bar{\mu} > 0$  it is easy to see, from the dynamics of (1), that the trajectory has to leave this set in finite time. This time depends on  $S_h, S_l$  and as  $(S_h - S_l) \to 0$  it coincides with the optimal one, i.e.  $T(F_{app}, S_l, S_h, z_0) \to T_{opt}(z_0)$ , and therefore  $\Delta(S_l, S_h) \to 0$ .

An explicit expression for  $\Delta(S_l, S_h)$  is complicated and will not be given here (see [7] for more details). However, a rough calculation is the following: the time the optimal control spends in the set  $S_l \leq S \leq S_h$  is approximately proportional to  $1/\mu^*$ , whereas the one spent by the suboptimal one is almost proportional to  $1/\bar{\mu}$ , with  $\bar{\mu} = \min(\mu(S_l), \mu(S_h))$ . Therefore  $\Delta(S_l, S_h)$  is roughly proportional to  $(1/\bar{\mu} - 1/\mu^*)$ . Note that the suboptimal control law is robust against model and parameter uncertainties and/or changes. Moreover, it requires little information from the system: only S needs to be measured and  $S^*$  and the instant when  $V = V_f$  need to be known.



Figure 2: Event Driven Time Optimal Control scheme

Tag	Trigger	Estimation	Meaning
$e_{1.0}$	$d\gamma/dt \le 0$	$S < S^*$	Not inhibited
$e_{2.1}$	$\gamma \le P\gamma_k^*$	$S = S_h$	Must wait
$e_{1.2}$	$\gamma \le P\gamma_k^*$	$S = S_l$	Must fill
$e_3$	$V \ge V_f$	(measured)	Tank full
$e_4$	$\gamma < \gamma_{\rm end}$	$S < S_{\min}$	End of reaction

Table 1: ESS events for fed-batch processes

### **3.2.2** Robust Suboptimal control law using $f(\mu)$ (ED-TOC)

Since S is not available, the previous control cannot be implemented. In this section it will be shown that, when instead of S a strictly monotonic increasing and continuous but unknown function of  $\mu$  is available, i.e.  $\gamma = f(\mu)$ , as for example  $f(\mu) = (a\mu + b)c$ , for a, b, c unknown constants, a, c > 0, it is possible to derive a control law that approximates arbitrarily well the optimal one. The motivation for this is that h(X, S, V) in (9), that can be calculated using measured signals through (8), is such a function, when the total biomass B is assumed constant. This is a good approximation for WWTPs. The approximate optimal control law (12) can be realized using the signal  $\gamma$ , as illustrated in Figure 2. First an Events Software Sensor (ESS) extracts from signal  $\gamma$ the occurrence of some *events*, that change the state of the Event Driven Time Optimal Controller (ED-TOC), a finite state machine that provides the control actions for the influent pump. Table 1 shows the events estimated by the ESS, and the finite state ED-TOC is depicted in Figure 3.



Figure 3: Finite State Transitions for ED-TOC

To understand the ESS consider the maximum  $\gamma^* = \max_{S \ge 0} f(\mu(S)) = f(\mu^*)$ , and that a value 0 < P < 1 of the near-optimality control parameter, has been selected. In what follows it will be assumed that  $\gamma^*$  is constant. The limits of the interval  $S_l \le S \le S_h$ , where the trajectory has to be maintained by the controller, are defined by the equations  $f(\mu(S_l)) = f(\mu(S_h)) = P\gamma^*$ . Making P close to one renders  $S_l$ ,  $S_h$  close to  $S^*$ . Figure 1 shows the relation between  $S_l$ ,  $S_h$ ,  $\gamma^*$  and P for the case  $\gamma = f(\mu) = (a\mu + b)c$ . If Assumption 1 is satisfied with  $\hat{S} > S_h$ , and because the monotone increasing (decreasing) behavior of S(t) when it goes from  $S_l$  to  $S_h$  (from  $S_h$  to  $S_l$ , respectively), it is clear that  $\gamma(t)$  increases from  $\gamma_l = f(\mu(S_l))(\gamma_h = f(\mu(S_h)))$  until maximum  $\gamma^*$  and then decreases until  $\gamma_h$  ( $\gamma_l$  respectively) (see Figure 1).

The initial state of the ED-TOC at k = 0 for  $t = t_0 = 0$  is always  $\sigma_0$  (see Fig. 3), for which  $F_{in} = 0$ . If the plant initial state S(0) is such that  $S(0) > S^*$  then S(t) decreases and  $\dot{\gamma}(t) > 0$  until  $S^*$  is reached. After that  $\dot{\gamma}(t) < 0$ , indicating that  $S < S^*$  and the ESS produces the event  $e_{1.0}$  (see Table 1) and the ED-TOC switches to the state  $\sigma_1$  (see Fig. 3), where  $F_{in} = F_{\text{max}}$ . If  $S(0) < S^*$  then this transition occurs immediately. In this state  $\gamma(t)$  increases until  $\gamma^*$  and then decreases. When S(t) reaches  $S_h$ ,  $\gamma(t) = P\gamma^*$  and the event  $e_{2.1}$  is produced by the ESS (see Table 1) and the ED-TOC switches to the state  $\sigma_2$  (see Fig. 3), where  $F_{in} = 0$ . Note that the detection of  $e_{2.1}$ 

requires the knowledge of  $\gamma^*$ . To avoid this, i.e. if  $\gamma^*$  is unknown, the ESS estimates a maximum of  $f(\mu)$  in real time, as  $\gamma_{\kappa}^*(t) = \max_{\tau \in (t_k, t)} f(\mu(S(\tau)))$  for  $\tau \in (t_k, t)$ , were  $t_k$  is the instant when the last k-th state change in the ED-TOC took place. Being in  $\sigma_2$  the S(t) decreases and  $\gamma(t)$  increases until  $\gamma^*$  and then decreases. When S(t) reaches  $S_l$ ,  $\gamma(t) = P\gamma^*$  and the event  $e_{1,2}$  is produced by the ESS (see Table 1) and the ED-TOC switches to the state  $\sigma_1$  (see Fig. 3). A cycling between  $\sigma_1$  and  $\sigma_2$  will happen until the tank is filled, where the event  $e_3$  will take place and the state  $\sigma_3$  will be reached. The reaction finishes when event  $e_4$  is produced and the state  $\sigma_4$  is reached. After this the rest of the batch sequence (settling, draw...) may be completed and afterwards a whole new cycle may be started. It should be noted that the ED-TOC does not require the knowledge of the exact shape of  $\mu$  or  $f(\mu)$ , or the values of  $\gamma^*$ ,  $S_l$  or  $S_h$  to operate correctly. For this control strategy a result similar to Theorem 3 applies.

**Theorem 4** Suppose that system (1) is given, that a continuous and strictly monotone increasing function  $f(\mu)$  of  $\mu$  is available, and Assumption 1 is satisfied with  $\hat{S} > S_h$ . Assume, furthermore, that  $\gamma^*$  is constant for each batch cycle, but unknown. Then replacing the optimal control law (10) by the ED-TOC law the time to reach the target from any initial condition  $\mathbf{z}_0 \in \Omega$  is

$$T_{EDTOC}(P, \mathbf{z}_0) = T_{opt}(\mathbf{z}_0) + \Delta(P) + \delta$$
(14)

with  $\Delta(P)$  continuous and finite and  $\Delta \to 0$  as  $P \to 1$ , i.e. the target will be reached in finite time, as near to the optimal one as desired, up to a small value  $\delta \ge 0$ , depending on the test state  $\sigma_0$ . This is true for any form of the growth rate (positive if S positive), of the function  $f(\mu)$ , for unknown  $S_{in}$  and for any value of the parameter  $Y_{X/S}$ .

**Proof.** Since the ED-TOC is simply a realization of the same control law of the previous Theorem 3 using  $\gamma(t)$  instead of S(t), the main part of the proof is identical to the proof of the previous

Theorem. The value  $\delta \geq 0$  is introduced by the initial test (Figure 3) when  $S(0) < S^*$ , since in this case during the the time it takes the ESS to determine the first event the wrong input  $F_{in} = 0$  will be applied. Although theoretically  $\delta = 0$ , in practice a positive value is preferred to let the signals stabilize. The robustness derives from the fact that the ESS can estimate correctly the events even if low information on the plant is known.

Note that the approximate control law is robust against model and parameter uncertainties and changes. Moreover, it requires low information from the system: only  $\gamma = f(\mu)$  and the instant when  $V = V_f$  have to be known, and the finishing value  $\gamma_{\min}$  given. It is important to note that the trajectory converges to the set  $S_l \leq S \leq S_h$  independently of and without knowledge of the parameters, the exact form of the growth rate, of  $f(\mu)$  and of the value of  $S_{in}$ .

## 3.3 Robust general near-optimal control law

In the previous paragraph the ED-TOC, a time suboptimal control law, was introduced. If estimations in Table 1 are exact, the reaction time of the ED-TOC can be made as near to time optimality as desired by selecting appropriately the parameter P. However, this property depends strongly on the availability of an exact value for  $\gamma$ . If there is some measurement noise or perturbation, if the parameters vary in time or as function of some other state variables, then Theorem 4 is no longer valid as estimations in Table 1 might have errors. In this Section it will be shown that, under reasonable circumstances, the estimation errors are tolerably low and so the approximated control still behaves correctly and robustly. The tradeoff is that optimality cannot be arbitrarily well approximated.

In particular, the case will be considered when the practically possible measurement  $\eta(t)$ , given by (9) for the system (1), is used in the ED-TOC instead of  $\gamma(t)$  in Figure 2 and Table 1. Note that h(X, S, V) is not in the form required by Theorem 4 when B is not supposed to be constant. However, the available signal  $\eta(t) = h(X(t), S(t), V(t))$  can be written in the form  $\eta = \gamma B$ , where  $\gamma = f(\mu)$  is a signal that satisfies the conditions of Theorem 4 to realize the ED-TOC. Since the total biomass B = XV satisfies  $\dot{B} = \mu B$ , it follows that  $B(t) = B(t_0) \exp\left(\int_{t_0}^t \mu(S(\tau)) d\tau\right)$ , i.e. it is a monotone increasing function of time. Recall that the operation of the ED-TOC based on  $\gamma(t)$  uses the fact that after  $\gamma(t)$  reaches its maximum value  $\gamma^*$  it decreases until the value  $P\gamma^*$ , when the control is switched. When  $\eta(t) = \gamma(t) B(t)$  is used in the ED-TOC the droop of  $\gamma(t)$  after reaching  $\gamma^*$  will not be followed by  $\eta(t)$  because of the increase of B(t), and the ED-TOC will not be able to correctly take a control decision using  $\eta(t)$  instead of  $\gamma(t)$ . However, if this masking effect is only temporary, and  $\eta(t)$  does reach a maximum  $\eta_{\text{max}}$  and then decreases until the value  $P\eta_{\text{max}}$ , then it is possible to use  $\eta(t)$  in the ED-TOC. The next Theorem gives sufficient conditions for this to happen.

To state the Theorem consider an "underlying" ED-TOC based on  $\gamma$  operating with a value  $0 < \bar{P} < 1$ , so that the conditions of Theorem 4 are satisfied. If  $\gamma^* = \max_{S \ge 0} f(\mu(S)) = f(\mu^*)$  the equations  $f(\mu(S_l)) = f(\mu(S_h)) = \bar{P}\gamma^*$  define the limits of the interval  $S_l \le S \le S_h$ . Define as  $T_h$  the maximum possible time to reach  $S_h$  initiating at  $S^*$  when  $F_{in} = F_{\max}$ . Similarly, assign  $T_l$  to the maximum possible time to reach  $S_l$  from  $S^*$  when  $F_{in} = 0$ , and denote  $T_{\max} = \max(T_h, T_l)$ . The basic idea of the following result is that if the biomass growth during  $T_{\max}$  is small enough, then  $\eta(t)$  will fall down, following  $\gamma(t)$ , and can be used instead of  $\gamma(t)$  in the ED-TOC (see Figure 2). If the parameter P in the ED-TOC (see Table 1) is selected as  $P = \bar{P} \exp(\mu^* T_{\max}) < 1$ , bigger than  $\bar{P}$ , then the behavior of the ED-TOC based on  $\eta$  is basically the same as that of the "underlying" ED-TOC based on  $\gamma$  with parameter  $\bar{P}$ . Let  $\varphi'$  represents the derivative of  $\varphi$  with respect to its argument.

**Theorem 5** Suppose that system (1) is given, with continuously differentiable  $\mu$ , and that  $\eta = f(\mu) B$  is available for measurement, with B the total biomass and  $f(\mu)$  a continuously differentiable and strictly monotone increasing function of  $\mu$ . Assume, furthermore, that  $\gamma^* = \max f(\mu)$  is

unknown, but constant, for each batch cycle. Suppose that  $\mu' > 0$  and that  $f - f'\mu'X_0 < 0$  when evaluated at S = 0, with  $X_0$  the initial biomass concentration in the reactor. Suppose a  $0 < \bar{P} < 1$ is selected, so that the conditions of Theorem 4 are satisfied, that the corresponding  $T_{\text{max}}$  is finite, that  $\bar{P} < \exp(-\mu^*T_{\text{max}})$  and that Assumption 1 is satisfied with  $\hat{S} > S_h$ . Under these conditions if, in Table 1,  $\gamma$  is replaced by  $\eta$ , and the parameter P is set to  $P = \bar{P} \exp(\mu^*T_{\text{max}})$ , then the ED-TOC law operates correctly and the time to reach the target from any initial condition  $\mathbf{z}_0$  is

$$T_{ROB}(P, \mathbf{z}_0) \le T_{EDTOC}(\bar{P}, \mathbf{z}_0) + \Xi , \qquad (15)$$

for some  $\Xi \geq 0$ .

**Proof.** Suppose that the ED-TOC is in  $\sigma_0$ , and therefore  $F_{in} = 0$ .  $\gamma_{inf} = f(\mu(0))$  is a lower bound for  $\gamma(t)$ . Along a trajectory of the plant

$$\dot{\eta} = (\dot{\gamma} + \mu f(\mu)) B = \left(-\frac{f'\mu'B}{V_0 Y_{X/S}} + f(\mu)\right) \mu B .$$
(16)

From (1) it is found that, when  $F_{in} = 0$ , then  $d\left(B + Y_{X/S}VS\right)/dt = 0$ , and therefore B at any time can be expressed as a function of S,  $B(t) = B_0 + Y_{X/S}V_0(S_0 - S(t))$ . Given the initial conditions  $\dot{\eta}$  in (16) is a function of S, and  $\dot{\eta}(S = 0) = 0$ , since  $\mu(0) = 0$ . Differentiating (16) with respect to S and evaluating at S = 0 gives  $d\dot{\eta}(0)/dS = \mu'B\left(f - \frac{f'\mu'B}{V_0Y_{X/S}}\right)\Big|_{S=0}$ . By hypothesis this quantity is negative, so that in a neighborhood of S = 0 the derivative  $\dot{\eta}$  becomes negative. Since for every value  $S \ge S^*$  the time derivative  $\dot{\eta} > 0$  (because  $\dot{S} < 0$ ) is positive, it follows that  $\dot{\eta}$  will become negative for some value  $S < S^*$ . And so for every initial condition of the reactor the ED-TOC will wait until  $\dot{\eta} \le 0$ , at some  $S < S^*$ , to go to the state  $\sigma_1$ , and this will occur in finite time.

Now assume that the ED-TOC is in state  $\sigma_1$ , and  $S < S^*$ . Since  $F_{in} = F_{max}$  the substrate S will increase, and it will take the values  $S(t^*) = S^*$  and  $S(t^* + t_h) = S_h$ , for some positive  $t^*$ ,  $t_h$ .

Correspondingly,  $\gamma(t)$  will grow until  $\gamma(t^*) = \gamma^*$  and then decrease until  $\gamma(t^* + t_h) = \bar{P}\gamma^*$ . The behavior of  $\eta(t)$  is such that it will increase until  $\eta(t^*) = \gamma^* B(t^*)$  and then it will reach  $\eta(t^* + t_h) = \bar{P}\gamma^* B(t^* + t_h)$ . However, it is not clear that  $\eta(t^* + t_h) < \eta(t^*)$ , since B(t) is increasing. But since its increment is bounded by  $B(t) \leq B(t^*) \exp(\mu^*(t - t^*))$ , it follows that

$$\eta(t^* + t_h) \le \bar{P}\gamma^* B(t^*) \exp(\mu^* t_h) = \bar{P} \exp(\mu^* t_h) \eta(t^*)$$
.

If  $\bar{P} \exp(\mu^* t_h) < 1$  then  $\eta(t^* + t_h) < \eta(t^*)$  and the maximum of  $\eta(t)$  will be reached in the interval  $t \in [t^*, t^* + t_h]$ . If the parameter P of the ED-TOC is such that  $1 > P \ge \bar{P} \exp(\mu^* t_h)$ , then the control will switch before  $S_h$  has been reached.

When the ED-TOC is in state  $\sigma_2$ , and  $S > S^*$ ,  $F_{in} = 0$  and the substrate S will decrease reaching  $S(t^*) = S^*$  and  $S(t^* + t_l) = S_l$ , for some  $t^*, t_l > 0$ . Correspondingly,  $\gamma(t)$  will grow until  $\gamma(t^*) = \gamma^*$  and then decrease until  $\gamma(t^* + t_l) = \bar{P}\gamma^*$ . The same previous analysis shows that if  $\bar{P} \exp(\mu^* t_l) < 1$  then  $\eta(t^* + t_l) < \eta(t^*)$  and the maximum of  $\eta(t)$  will be reached in the interval  $t \in [t^*, t^* + t_l]$ . If the parameter P of the ED-TOC is such that  $1 > P \ge \bar{P} \exp(\mu^* t_l)$ , then the control will switch before  $S_l$  has been reached. Note that the previous analysis shows that when the ED-TOC is in  $\sigma_0$ , and the initial condition is  $S_0 \ge S^*$ , the ED-TOC will go to state  $\sigma_1$  before  $S_l$ has been reached.

The values  $t_h$  and  $t_l$  depend on the particular trajectories. If there exist  $T_h = \sup \{t_h\}$ , and  $T_l = \sup \{t_l\}$ , i.e. upper bounds for all possible transit times, then if  $\bar{P} \exp(\mu^* T_l) < 1$  and  $\bar{P} \exp(\mu^* T_h) < 1$  it is possible to select  $1 > P \ge \bar{P} \exp(\mu^* T_{\max})$ , where  $T_{\max} = \max \{T_l, T_h\}$ , so that the ED-TOC will cycle between  $\sigma_1$  and  $\sigma_2$ , and the substrate will be confined in the region  $S_l \le S \le S_h$ . When the tank is full the ED-TOC will go to state  $\sigma_3$ , where  $\eta(t)$  will finally decrease until the end condition  $\eta \le \eta_{\text{end}}$  has been reached and the ED-TOC switches to state  $\sigma_4$ .

The inequality (15) is the result of two facts. First that the proposed control law assures that

 $S_l \leq S \leq S_h$ , and therefore  $T_{\text{EDTOC}}(\bar{P}, \mathbf{z}_0)$  is an upper bound for the reaction time. Second, the term  $\Xi$  is introduced by the extra delay in the test and the end phases of the ED-TOC.

It follows from (15) that, except for the term  $\Xi$ , that can be small, the reaction time for the ED-TOC based on  $\eta$  is smaller than that of the ED-TOC based on  $\gamma$ . To complete the previous Theorem, in the next Lemma explicit bounds for  $T_{\text{max}}$  will be given, in terms of some parameters of the plant. Note that  $T_{\text{max}}$  depends on the selected value of  $\bar{P}$ .

Lemma 6 Define the parameters

$$\beta \triangleq \frac{F_{\max} Y_{X/S}}{B_M \mu^*} \left( S_{\inf} - S_h \right) \ , \ \varrho \triangleq \frac{Y_{X/S}}{X_M} \left( S_h - S^* \right) \ , \tag{17}$$

where  $S_{inf}$  is the minimum value of  $S_{in}(t)$ , during the relevant time interval,  $X_M$  is the maximum biomass concentration in the reactor, and  $B_M = X_M V_f$ . If  $\rho > 0$  the equation

$$1 - \exp\left(\mu^* T_h\right) + \beta \mu^* T_h = \varrho \tag{18}$$

has non negative solutions  $T_h$  if and only if the inequalities

$$\beta > 1 , \ 0 < \varrho \le 1 + \beta \left( \ln \beta - 1 \right) \tag{19}$$

are fulfilled. Moreover, there is exactly one solution in the interval  $0 \le \mu^* T_h \le \ln \beta$ . Let  $T_l$  be given by the expression

$$T_l = \frac{(S^* - S_l) V_f Y_{X/S}}{\mu(S_l) B_0} , \qquad (20)$$

where  $B_0$  is the initial total biomass in the reactor. Then  $T_{\text{max}} = \max(T_h, T_l)$  is finite.

**Proof.** Consider first that  $F_{in} = 0$ ,  $S = S^*$ , and that the biomass concentration is X. Since

S decreases it will be in the interval  $S \in [S_l, S^*]$ , where the minimal degrading rate is  $\mu_l = \mu(S_l)$ . And so S has to reach  $S_l$  in a maximal time given by  $t_l = \frac{(S^* - S_l)Y_{X/S}}{\mu_l X}$ . An upper bound  $T_l$  for  $t_l$  is therefore given by (20). Consider now that  $F_{in} = F_{\max}$ ,  $S = S^*$ , that the biomass concentration is  $\bar{X}$ , and that the volume is  $\bar{V}$ . From (1) it follows that  $d(VS)/dt = -\frac{\mu B}{Y_{X/S}} + F_{\max}S_{in}, V(t) = \bar{V} + F_{\max}t,$ and  $B = \mu B$ . A lower bound for the growth of VS is obtained taking in the previous equations the maximum value of  $\mu = \mu^*$ , and the minimum value of  $S_{in} = S_{inf}$ . An upper bound for B is B(t) = $\bar{B}\exp(\mu^*t)$ , with  $\bar{B}=\bar{V}\bar{X}$ , and a lower bound Z for S is found solving the differential equation  $d(VZ)/dt = -\frac{\mu^* \bar{B} \exp(\mu^* t)}{Y_{X/S}} + F_{\max} S_{\inf}.$  Integrating for  $t \in [0, t_h]$ , and considering that  $Z(t_h) = S_h$ ,  $Z(0) = S^* \text{ it is obtained } \left(\bar{V} + F_{\max}t_h\right)S_h = S^*\bar{V} + \bar{B}\left(1 - \exp\left(\mu^*t_h\right)\right)/Y_{X/S} + F_{\max}S_{\inf}t_h. \text{ Therefore a state of the set of th$ an upper bound  $T_h$  for  $t_h$  can be found solving the equation (18). Set  $T \triangleq \mu^* T_h$ , and the left hand side of (18) as the function  $g(T) \triangleq 1 - \exp(T) + \beta T$ . Note that g(0) = 0,  $\lim_{T \to \infty} g(T) = -\infty$  and  $g'(T) = -\exp(T) + \beta$  is a monotone decreasing function. If  $\beta \leq 1, g(T) \leq 0$  for all  $T \geq 0$ . If  $\beta > 1$ , g(T) grows monotonically in the interval  $T \in [0, \ln \beta]$ , reaches a maximum  $g(\ln \beta) = 1 - \beta + \beta \ln \beta$ at  $T = \ln \beta$  and decreases monotonically for  $T > \ln \beta$ . If  $\rho = 0$ , T = 0 is a solution of (18) for every  $\beta$ . For  $\rho > 0$  it is then necessary and sufficient that inequalities (19) are satisfied for the existence of a positive solution for T. In this case two solutions exist, and the smaller one satisfies  $T \leq \ln \beta$ . Note that the first condition in (19) assures that S can reach  $S_h$ .

The calculation of feasible values of  $\bar{P}$  in Theorem 5 can be made recursively: set  $\bar{P}$  and calculate  $T_{\max}$  using Lemma 6, and then check if the expression  $\bar{P} < \exp(-\mu^* T_{\max})$  is satisfied. Alternatively, the last expression is an implicit inequality for  $\bar{P}$ , since  $T_{\max}$  is a function of  $\bar{P}$ . In general no much can be said about its solution set. There are several possibilities, as for example that there is no  $\bar{P}$  or that only values of  $\bar{P}$  much smaller than 1 satisfy the inequality. In the first case the ED-TOC based on  $\eta$  cannot be assured to operate, and in the second one its reaction time can be very far away from the time optimality. In fact it can be shown that time optimality cannot be arbitrarily

set by any ED-TOC based on  $\eta$ .

**Lemma 7** Suppose that conditions (19) in Lemma 6 are satisfied for some  $\bar{P}^* \in [0,1]$ . Then it follows that  $\bar{P} \exp(\mu^* T_{\max}(\bar{P})) > 1$  in some interval  $\bar{P} \in (\bar{P}_{\max}, 1)$ .

**Proof.** Consider the function  $r(\bar{P}) \triangleq \bar{P} \exp(\mu^* T_{\max}(\bar{P}))$ . The function is continuous for  $\bar{P} \in [0,1]$ , since  $S_l(\bar{P})$  and  $S_h(\bar{P})$  are continuous, and so are  $T_l(\bar{P})$  and  $T_h(\bar{P})$  as solutions of (20) and (18), respectively. Moreover, r(1) = 1 since  $T_{\max}(1) = 0$ . It will be shown that  $r(\bar{P}) > 1$  in some interval  $\bar{P} \in (\bar{P}_{\max}, 1)$ . This will be done by taking the derivative of  $r(\bar{P})$  and showing that it is negative for values of  $\bar{P}$  to the left of 1, where it is defined. Where it exists  $r'(\bar{P}) = (1 + \mu^* \bar{P}T'_{\max}(\bar{P})) \exp(\mu^* T_{\max}(\bar{P}))$ .  $T'_{\max}(\bar{P})$  is either  $T'_h(\bar{P})$  or  $T'_l(\bar{P})$ , where it is defined. From (20), (18), (17) and  $f(\mu(S_l)) = f(\mu(S_h)) = \bar{P}\gamma^*$  one obtains

$$\begin{split} T'_{l}\left(\bar{P}\right) &= -\frac{V_{f}Y_{X/S}}{B_{0}}\frac{\left[\mu\left(S_{l}\right) + \left(S^{*} - S_{l}\right)\mu'\left(S_{l}\right)\right]}{\mu^{2}\left(S_{l}\right)}S'_{l}\left(\bar{P}\right) \ ,\\ \varrho'\left(\bar{P}\right) &= \frac{Y_{X/S}}{X_{M}}S'_{h}\left(\bar{P}\right) \ , \ \beta'\left(\bar{P}\right) &= -\frac{F_{\max}Y_{X/S}}{B_{M}\mu^{*}}S'_{h}\left(\bar{P}\right) \ ,\\ T'_{h}\left(\bar{P}\right) &= \frac{\frac{Y_{X/S}}{X_{M}} + T_{h}\left(\bar{P}\right)\frac{F_{\max}Y_{X/S}}{B_{M}}}{\mu^{*}\left[\beta\left(\bar{P}\right) - \exp\left(\mu^{*}T_{h}\left(\bar{P}\right)\right)\right]}S'_{h}\left(\bar{P}\right) \ ,\\ S'_{l}\left(\bar{P}\right) &= \frac{\mu^{*}}{f'\left(\mu\left(S_{l}\right)\right)\mu'\left(S_{l}\left(\bar{P}\right)\right)} \ , \ S'_{h}\left(\bar{P}\right) &= \frac{\mu^{*}}{f'\left(\mu\left(S_{h}\right)\right)\mu'\left(S_{h}\left(\bar{P}\right)\right)} \end{split}$$

where this derivatives are defined. Since from (19)  $\beta > 1$ ,  $\beta(\bar{P}) - \exp(\mu^*T_h(\bar{P})) > 0$  for  $\bar{P}$  near to 1. It is clear that these derivatives are not defined for  $\bar{P} = 1$ . But since  $S'_l(\bar{P}) > 0$  for  $\bar{P} \in [0, 1)$ and  $\lim_{\bar{P}\to 1^-} S'_l(\bar{P}) = \infty$ , and  $S'_h(\bar{P}) < 0$  for  $\bar{P} \in [0, 1)$  and  $\lim_{\bar{P}\to 1^-} S'_h(\bar{P}) = -\infty$ , it follows that  $T'_l(\bar{P}) < 0$  and  $T'_h(\bar{P}) < 0$  for  $\bar{P} \in [0, 1)$  and  $\lim_{\bar{P}\to 1^-} T'_h(\bar{P}) = \lim_{\bar{P}\to 1^-} T'_l(\bar{P}) = -\infty$ . Since  $r(\bar{P})$  is continuous this implies that  $r(\bar{P}) > 1$  in some interval  $\bar{P} \in (\bar{P}_{\max}, 1)$ .

The interpretation of this Lemma is that for every ED-TOC based on  $\eta$  there is a pay-off: the reaction time cannot be better than that one obtained using  $\gamma$  with  $\bar{P} = \bar{P}_{\text{max}}$ .

However, there is a condition, satisfied in practical applications (see the Experimental results in the next Section), for which the full performance of the ED-TOC based on  $\gamma$  is nearly recovered when  $\eta$  is used. This is the case since  $\bar{P}_{\text{max}} \approx 1$ , and so there is no important loss of time optimality.

**Corollary 8** Consider that the conditions of Theorem 5 and Lemma 6 are satisfied. Then  $\bar{P}_{max}$  is near to 1 if  $F_{max}$  or  $S_{inf}$  and  $B_0/V_f$  are large enough.

**Proof.** Set a desired value of  $\bar{P}_{max}$ . This fixes the values of  $S_l$  and  $S_h$ . From  $\bar{P}_{max} \exp(\mu^* T_{max}(\bar{P}_{max})) = 1$  an upper bound for  $T_{max}(\bar{P}_{max})$  is obtained. The solution  $T_h$  of (18) can be upper bounded by  $\varrho/(\mu^*(\beta - k))$  for some k > 0. From this last expression and equation (20) the conclusion follows easily.

If the conditions of Corollary 8 are robustly satisfied, i.e. for the whole family of plant models, then the ED-TOC based on  $\eta$  is similar to the ED-TOC based on  $\gamma$  and the results of Theorem 4 are recovered, i.e. the ED-TOC based on  $\eta$  is robust and can be brought very near to time optimality. Note that the previous Lemmata and the Corollary can be used to design the parameters of the process, so that the control strategy operates correctly.

**Remark 9** In the next section experimental results for a WWTP ([2]) are presented. The successful operation of the ED-TOC can be interpreted using the analysis in this section, and in particular in the Corollary 8. Alternatively, they can be also understood using the results in Section 3.2.2 since the change in B during one cycle is so small that it can be practically considered as constant. This is the case, since the amount of toxic that can be treated is small compared to  $B_0$ . Although the analysis in this paper has been limited to an application in WWTP, the results can be applied to some biotechnological processes. In this case the change in B is usually large. Even for such a case simulation results show the effectiveness of the ED-TOC [3].

Remark 10 No noise analysis has been carried out but it can be done in a similar fashion as the

proof of Theorem 5.

**Remark 11** In practice, derivatives for Equation (6) and Table 1 are not available. They are calculated using numerical real-time methods. This introduces some time delays and distortion in the derivative signal. The same is true for signals generated using real practical sensors devices. A way to deal with such time delays is given in [2]. Distortions could be treated theoretically in the same way as noise.

**Remark 12** When the specific growth rate  $\mu(S)$  is of monotonic-type (non-inhibitory), then the TOC consists in setting  $F_{in} = F_{max}$  until the reactor is full, and then applying  $F_{in} = 0$  until  $S \leq S_{min}$ . When the ED-TOC is applied to such a process, it behaves as expected from the TOC. The same is true if Assumption 1 is not satisfied for any  $\hat{S} > S^*$ . In this case the TOC and the behavior of the ED-TOC is the one of a bioreactor with a Monod-type specific growth rate.

## 4 Experimental results

A 7 L laboratory scale bioreactor acclimated with sludge taken from a municipal WWTP was used to degrade 4-chlorophenol (4CP). The usual influent toxicant concentration for traditional sequencing batch processing is  $S_{in} = 350 \text{ mg4CP/L}$ . Applying more than twice such quantity would greatly inhibit and stress the biomass, increasing the needed treating time nonlinearly. Applying higher toxicant concentrations might even inhibit and/or disable the bioreactor permanently. By using the ED-TOC strategy, instead, the biomass was never stressed or inhibited. A linear increase relation of treating time with respect to  $S_{in}$  was observed in a series of experiments for increasing  $S_{in}$ , even when making it as high as 7000 mg4CP/L. Theoretically, treating time was near 95% of the optimal-time, in all series, for a programmed P = 0.9

Figure 4 shows one experimental kinetic for the 4CP degradation case, using  $\eta(t)$  in Equation



Figure 4: Experimental kinetics using ED-TOC in WWTP. Operating Parameters P = 0.9; influent toxicant concentration  $S_{in} = 428 \text{ mg4CP/L}$ 

(8) for ED-TOC implementation. Toxicant substrate concentration S inside the bioreactor (see 4CP in Figure 4, triangular marks) was measured off-line from manually taken samples and was not used for control purposes. Up to S = 200 mg4CP/L it is considered normal and safe for the biomass. A model identification exercise later revealed a 95% confidence interval of  $\pm 7.4\%$  for  $S^* = 13.99 \text{ mg4CP/L}$ . Figure 4 shows that S was kept oscillating around  $S^*$ , in an acceptably low concentration range, by properly turning on and off the influent pump (Figure 4, dotted line). Such behavior shows the effectiveness of the ED-TOC strategy.

Biomass was  $B_0 = 1.4$  g exhibiting an increase of less than 2% during the reaction. Its value was not used by the controller. Values of S,  $S_{in}$  and  $S^*$  were not used either. Another perturbation comes from the online sensor used to measure Dissolved Oxygen (Figure 4, continuous line). It introduced appreciable second order delay effects, and some noise, to the state variable O. It follows that some delays and signal distortion are to be expected when calculating  $\eta$  (Figure 4, discontinuous line) in (8) for using it in ED-TOC. But thanks to ED-TOC robustness the system did cope smoothly with all this perturbations and uncertainties.

# 5 Conclusions

A methodology for the robust and practical implementation of optimal control strategies for a class of nonlinear processes has been introduced. When the control law is composed of bang-bang and singular arcs the basic idea is to replace the singular arc with a bang-bang control. This makes the control robust and requires a reduced quantity of information. This general idea is developed here for a class of fed-batch bioreactors, in particular for its application to Waste Water Treatment, although the control law can also be applied in biotechnology.

The use of measurable variables giving minimal indirect information is shown to be effective for software-sensing events related to the crossing of the singular surface of the process. This allows the controller to generate bang-bang cycles to approximate the singular arcs of the optimal solution.

Experimental results in a laboratory scaled bioreactor for the treatment of toxic organic substances demonstrate the applicability of the proposed control strategy in a real system.

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# References

 G. Bastin and D. Dochain. On-line Estimation and Adaptive Control of Bioreactors, volume 1 of Process Measurement and Control. Elsevier, Amsterdam, 1990.

- [2] M.J. Betancur, J. Moreno, and G. Buitron. Event-driven control for treating toxicants in aerobic sequencing batch bioreactors. In Proc. of the 9th Intern. Symposium of Computer Applications in Biotechnology (CAB9), volume CDROM file 1074, 2004.
- [3] M.J. Betancur, M. Titica, J. Moreno, D. Dochain, and M. Guay. Event software sensor and adaptive extremum seeking alternatives for optimizing a class of fed-batch bioreactors. In Proceedings of 7th (IFAC) International Symposium on Dynamics and Control of Process Systems (DYCOPS), volume CDROM Paper 162.pdf, 2004.
- [4] H. Hermes and J.P. LaSalle. Functional analysis and time optimal control. Academic Press, N.Y., 1969.
- [5] H.K. Khalil. Nonlinear Systems. Prentice-Hall, Upsaddle River, New Jersey, third edition, 2002.
- [6] N. Marcos, M. Guay, D. Dochain, and T. Zhang. Adaptive extremum-seeking control of a con-tinuous bioreactor. J. Proc. Cont., 14(3):317–328, 2004.
- [7] J. Moreno. Optimal time control of bioreactors for the wastewater treatment. Optimal Control, Applications and Methods, 20:145–164, 1999.
- [8] D. Sarkar and J.M. Modak. Optimisation of fed-batch bioreactors using genetic algorithms. Chemical Engineering Science, 58:2283–2296, 2003.
- [9] K. Schügerl. Bioreaction Engineering, volume 1. John Wiley & Sons, Chichester, 1987.
- [10] J.J. Slotine and W. Li. Applied nonlinear control. Prentice Hall, Englewood Cliffs, N.J., 1991.
- [11] I.Y.M. Smets, K.J.E. Versyck, and J.F.M. Van Impe. Optimal control theory: a generic tool for identification and control of (bio-)chemical reactors. *Annual Reviews in Control*, 26:57–73, 2002.

- [12] M. Titica, D. Dochain, and M. Guay. Adaptive extremum-seeking control of fed-batch bioreactors. *European J. of Control*, 9:614–627, 2003.
- [13] J.F.M. Van Impe. Optimal control of fed-batch fermentation processes. In J. Van Impe, P. Vanrolleghem, and D. Iserentant, editors, Advanced Instrumentation, Data Interpretation, and Control of Biotechnological Processes, pages 319–346. Kluwer Acad. Pub., Dordrecht-Boston-London, 1998.
- [14] J.F.M. Van Impe and G. Bastin. Optimal adaptive control of fed-batch fermentation processes. Control Eng. Pract., 3(7):939–954, 1995.