

# EVENT SOFTWARE SENSOR AND ADAPTIVE EXTREMUM SEEKING ALTERNATIVES FOR OPTIMIZING A CLASS OF FED-BATCH BIOREACTORS

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**Abstract:** Optimization and control in spite of plant uncertainties is always a challenge, especially if additional constraints about measurements are present. Here, two different approaches to solve this problem are compared using simulation. They aim at reducing the operation time of bioreactors with inhibitory behavior where measuring the reaction rate is not feasible. The “Adaptive Extremum Seeking” proposed version relies on the structure information of the kinetic model and requires the measurements of the substrate and one other related variable. The “Event Driven Time Optimal Controller” strategy avoids the substrate measurement and, using an event software sensor, provides a nearly optimal solution without requiring a complete model. *Copyright © 2004 IFAC*

**Keywords:** Extremum seeking, software sensor, optimal control, fed-batch bioreactor, Haldane kinetics, control applications, biomass production

## 1. INTRODUCTION

The performance of fed-batch fermentation processes could typically be increased by the use of model-based optimization techniques. Using a fairly general model structure, many useful results have been derived in (Modak et al., 1986; Van Impe et al., 1994). One key result is that, in many cases, the final product yield (ratio of the amount of product formed and the amount of substrate consumed) can be maximized simply by maximizing the instantaneous yield. This can be achieved by maintaining the substrate concentration at an optimal level called  $S^*$ .

Over the past years, significant research effort has been done in the real time optimization for fed-batch bioreactors. The primary objective has been to overcome the performance limitations associated with the large uncertainty related to models of these processes (e.g. Bastin and Dochain, 1990).

In this paper, two approaches that are aimed at handling the uncertainties on the process kinetics are comparatively investigated. The version of the Adaptive Extremum Seeking (AES) proposed here utilizes explicit structure information of the objective function that depends on system states and unknown plant parameters. A Lyapunov-based adaptive control technique is used to estimate the unknown kinetic parameters and to drive the system to its unknown extremum. The second approach, the Event Driven Time Optimal Control (ED-TOC) uses bang-bang techniques based on the optimal solution approach, solving the problem without measuring the substrate nor needing the exact structure of the model.

The paper is organized as follows: in Section 2 the problem is stated. Sections 3 and 4, respectively, present the ED-TOC and the AES. A comparative simulation study is done in Section 5. Some conclusions and perspectives close the paper.

## 2. PROBLEM FORMULATION

In this work, we consider the optimization problem for a class of simple microbial growth processes with one gaseous product in a fed-batch bioreactor, described by the following dynamical model:

$$\frac{dX}{dt} = \mu X - DX \quad (1)$$

$$\frac{dS}{dt} = -k_1 \mu X + D(S_i - S) \quad (2)$$

$$y = k_2 \mu X \quad (3)$$

$$\frac{dV}{dt} = DV \quad (4)$$

where states  $X$  (g/L) and  $S$  (g/L) hold for biomass and substrate concentrations, respectively,  $\mu$  ( $h^{-1}$ ) is the specific growth rate,  $D = \frac{F}{V}$  ( $h^{-1}$ ) is the dilution rate,

$y$  (g/L/h) is the production rate of the reaction product,  $S_i$  (g/L) denotes the concentration of the substrate in the feed,  $k_1$  and  $k_2$  are yield coefficients,  $F$  (L/h) is the inflow and  $V$  (L) is the volume of the liquid medium in the tank.

A Haldane law approximates the specific growth rate:

$$\mu = \frac{\mu_0 S}{K_S + S + S^2 / K_I} \quad (5)$$

Where  $\mu_0$  is a parameter related to the maximum value of the specific growth rate  $\mu^*$ ,  $K_S$  denotes the saturation constant and  $K_I$  the inhibition constant. Such a model is typically used to describe the substrate inhibition effect in fed-batch bioreactors, as shown in Figure 1.

The control objective is to produce the maximum amount of biomass in the minimum possible time. It is well known (Moreno, 1999) that this will be achieved if  $\mu$  is kept at its maximum value,  $\mu^*$ , as shown in Figure 1.

## 3. EVENT DRIVEN TIME OPTIMAL CONTROL

The ED-TOC is based on the time optimal control solution to the problem (Moreno, J. 1999), which consists of bang-bang arcs and a singular arc. The

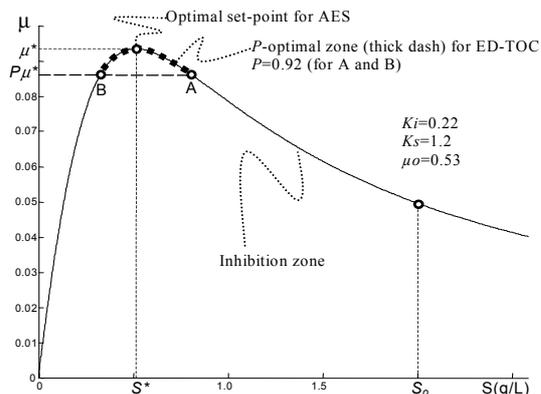


Figure 1. Haldane's type biomass specific growth rate

singular arc maintains  $\mu = \mu^*$  using a continuous control function, for which a good knowledge of the model would be required. The ED-TOC does the bang-bang arcs exactly but it approximates the singular arc by a switching strategy. This allows operating as near to the optimum as desired without the necessity of measuring many state variables and with a high degree of robustness against model and parameter uncertainties and changes. It considers also the physical restrictions of the actuator.

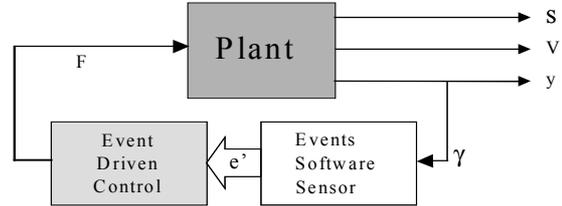


Figure 2. ED-TOC scheme

The ED-TOC estimates if  $\mu$  lies inside a  $P$ -optimal zone, depicted in Figure 1, and acts accordingly to keep it inside. Figure 2 shows the ED-TOC scheme (a formal description is available in Betancur et al. 2004). The main action applied to the manipulated variable  $F$  is on/off. This bang-bang action is determined using the estimated events  $e'$ . Basically the "Events Software Sensor" (ESS) generates two types of  $e$  events estimation. A parameter  $P \in (0,1)$  in Figure 1 tunes the points in  $\mu$  where real  $e$  are located. Event  $e=a$  means that  $S$  is definitely above  $S^*$  and that  $\mu$  is in the right-handed vicinity of point  $A$ , i.e.; moving away of the  $P$ -optimal zone. If the  $F$  pump is ON it must be turned OFF as shown in Figure 3. Similarly,  $e=b$  signals the moment in which the system is leaving the left border of the  $P$ -optimal zone, near point  $B$ . If  $F$  pump is OFF then it must be switched ON as shown in Figure 3. The final reaction's time  $t_f$  will be close to the optimal  $t_{fopt}$  as the established on/off cycle will keep the system as close as desired to  $\mu^*$  at all possible times, by properly choosing  $P \rightarrow 1$  (Table 1).

The ESS is called this way because, without measuring the variables  $\mu$  or  $S$  nor knowing the parameters  $(S^*, \mu^*)$ , it estimates  $e' \approx e$ , using a real-time software algorithm. For doing so a  $\gamma$  variable must be available, such that its shape is related to the shape of  $\mu$ , i.e. that as function of  $S$  its unique maximum coincides with  $S^*$ , regardless of other dependences it might have. For the case at hand  $\gamma$  is straightforwardly found in the gaseous product  $y$ :

$$\text{From (3): } \gamma = y(S, X) = k_2 \mu(S) X \quad (6)$$

It is evident from (6) that for a given unknown  $X > 0$  and any unknown  $k_2 > 0$  the shape of  $\gamma$  is the same as  $\mu$  in Figure 1. That is, they grow monotonically from  $S=0$  to  $S=S^*$ , and then they decrease, also monotonically, from  $S=S^*$  and beyond as  $S \rightarrow \infty$

But  $\gamma$  from (6) is useless as, except the fact they are positive, there is no available data for neither  $S$ ,  $X$  nor  $k_2$ . That is why the ESS uses the time format of  $\gamma$  in (3) as it can be measured online and its maximum is easily found at some special times. Let's define  $t_k^*$  as

the time when  $S$  just touches  $S^*$  for the  $k_{th}$  time. Then  $\gamma_k^* = \gamma(t_k^*)$  is a detectable maximum. Later an  $k_{th}$  estimated event  $e_k$  will be provided at time  $t_{ek}$  when  $\gamma(t_{ek}) = P\gamma_k^*$  indicating that the system is about to leave the  $P$ -optimal zone. Note that this algorithm works independently of the structure or form of  $\mu$  in (5), as long as it has a unique global maximum.

It should be noted in (3) that, as  $X(t)$  may change with time, a slight difference in the  $t_{ek}$  is expected compared to the situation if  $\mu$  were used directly instead of  $\gamma$ . This estimation inaccuracy decreases when  $X(t)$  varies slower than  $\mu(t)$ . Three cases of interest might arise. In the first, the influent pump is OFF and  $S$  decreases. It might happen that  $\gamma$  is increasing which means that the system is inhibited and above or in the vicinity of  $S^*$  (see left-side of Figure 3). Instead, if  $\gamma$  decreases, this means that the system is below  $S^*$ . The second case takes place when the pump is ON and sufficient substrate is being added to the tank as to increase  $S$  at some rate. Here, if  $\gamma$  is increasing, it means the system is "below" or in the vicinity of  $S^*$ . On the opposite, if  $\gamma$  decreases, this means that there is substrate inhibition, above  $S^*$ . The third case should be avoided. It is the limit case where  $S_i$  in  $F$  is not sufficient to guarantee that the increase in  $S$  will produce a  $\mu$  with a dynamics faster than that of  $X$ . This condition is easily avoidable, even if  $S_i$  changes over time, if the inflow provides significantly more substrate than would  $F_{opt}$ , the inflow needed for the optimal case (Moreno, 1999).

Figure 3 compares the behavior of the ED-TOC for two different values of  $P$ :  $P=P1=0.92$  corresponds to the Figure 1. The second case  $P=P2=0.998$  provides a much better efficiency at the detriment of the switching cycle for  $F$ . Table 1 summarizes the results for different values of  $P$ . There it can be seen that the switching time is reasonable for this application and that it can be enlarged, if necessary, accepting a small loss in optimality.

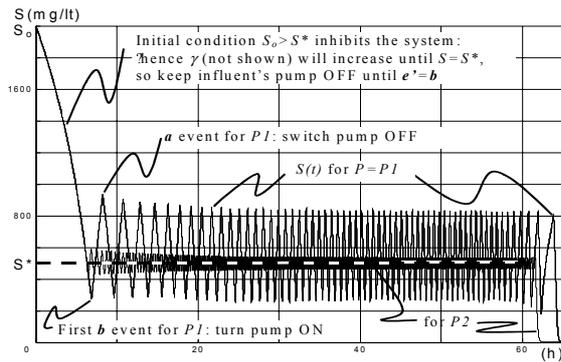


Figure 3. ED-TOC's Substrate kinetics for  $P1=0,92$  and  $P2=0,998$  shown together for comparison

Table 1 : ED-TOC optimality for different  $P$

$P$	Optimality index $t_{opt}/t_f$ [%]	$F$ pump cycles	Switching time [h]
0,998	99,9	448	0,14
0,98	99,8	151	0,41
0,96	99,2	106	0,59
0,90	96,0	62	1,0

#### 4.1. Principle and assumptions

The extremum-seeking scheme investigated here utilizes explicit structure information of the specific growth rate  $\mu$ . In the case of Haldane kinetics (5)  $\mu$  is maximum when the substrate concentrations equal to

$S^* = \sqrt{K_S \cdot K_I}$ . Then, the control objective is to keep the substrate concentration inside the reactor at the level  $S^*$ . Since the exact values of Haldane parameters are usually unknown (or at least poorly known), the adaptive extremum-seeking controller is developed to search this unknown set point such that the biomass production at the end of the reactor is maximized.

The adaptive extremum-seeking control scheme provides an adaptive control law of the dilution rate  $D$  to control the substrate  $S$  at the desired set point  $S^*$ , coupled with parameter learning laws for the Haldane model parameters. This algorithm requires the on-line knowledge of the substrate  $S$  and the gaseous outflow rate  $y$  (e.g.  $\text{CO}_2$ ), as well as the related yield coefficients.

*Parameter definition.* Let's define:

$$\theta_\mu = \frac{\mu_0}{K_S}, \quad \theta_S = \frac{1}{K_S}, \quad \theta_I = \frac{1}{K_S \cdot K_I} \quad (7)$$

$\theta = [\theta_\mu \quad \theta_S \quad \theta_I]^T$  represents the new set of kinetic parameters to be estimated on-line. The optimum for  $S$  can be re-expressed as follows:  $S^* = \frac{1}{\sqrt{\theta_I}}$ .

By this transformation, the optimum value is function of only one unknown parameter that has to be estimated on-line.

#### 4.2. Estimation and Controller Design

The controller design proceeds in different steps. First, the estimation equation for  $S$  is derived from the balance model equation, then the control law and the estimation of the unknown kinetic parameters are included in a Lyapunov based derivation framework.

*Estimation equation for the gaseous outflow rate  $y$*

By considering Eq. 1-3 and the kinetic parameter definition, the predicted state  $y$  is generated by:

$$\frac{d\hat{y}}{dt} = \frac{1 - \hat{\theta}_I S^2}{S(1 + \hat{\theta}_S S + \hat{\theta}_I S^2)} [D(S_i - S) - \theta_k y] y + \frac{\hat{\theta}_\mu S y}{1 + \hat{\theta}_S S + \hat{\theta}_I S^2} - D y + k_y e_y \quad (8)$$

with  $k_y > 0$  and  $e_y = y - \hat{y}$ .  $\theta_k = \frac{k_1}{k_2}$  is the ratio of the yield coefficients, assumed to be known.

### Design of the adaptive extremum-seeking controller

Since the parameter  $\theta_I$  is unknown, the desired set point (x) can be re-expressed as follows:  $S^* = \frac{1}{\sqrt{\hat{\theta}_I}}$ .

The controller is designed in order to drive the substrate concentration  $S$  to the estimated value of  $S^*$  (x). An excitation signal  $d(t)$  is designed and injected into the adaptive system such that the estimated parameter  $\hat{\theta}_I$  converges to its true value. The extremum seeking control objective can be achieved when the substrate concentration  $S$  is stabilized at the optimal operating set point  $S^*$ .

Define the error control variable  $z_S$  as follows:

$$z_S = S - \frac{1}{\sqrt{\hat{\theta}_I}} - d(t) \quad (9)$$

Consider the Lyapunov candidate function as follows:

$$V = \frac{z_S^2}{2} + \frac{1}{2} \left( \frac{\tilde{\theta}_\mu^2}{\gamma_\mu} + \frac{\tilde{\theta}_s^2}{\gamma_s} + \frac{\tilde{\theta}_I^2}{\gamma_I} \right) + \frac{e_y^2}{2} (1 + \theta_s \cdot S + \theta_I \cdot S^2) \quad (10)$$

where  $\tilde{\theta}_\mu = \theta_\mu - \hat{\theta}_\mu$ ,  $\tilde{\theta}_s = \theta_s - \hat{\theta}_s$  and  $\tilde{\theta}_I = \theta_I - \hat{\theta}_I$ ,  $\gamma_\mu, \gamma_s$  and  $\gamma_I$  are positive tuning parameters.

The adaptive extremum seeking controller algorithm is derived from the expression of the Lyapunov candidate function  $V$ , in such a way that  $\dot{V}$  is negative.

After mathematical manipulations, we obtain the control law and the parameter learning laws as follows:

Control law:

$$D = \frac{1}{S_i - S} [-k_z z_S + \theta_k y + a(t) - k_d d(t)] \quad (11)$$

Note that the resulting control law consists of two terms: the first one includes the specific rates of the biomass growth, while the second is a correcting term proportional to the error output and to the dither signal,  $d(t)$  defined as:

$$\dot{d}(t) = a(t) + \frac{1}{2} \cdot \hat{\theta}_I^{\frac{3}{2}} \cdot \frac{d\hat{\theta}_I}{dt} - k_d \cdot d(t) \quad (12)$$

where  $a(t)$  acts as a dither signal on the closed-loop process and  $k_d$  is a strictly positive constant.

Parameter learning laws

$$\frac{d\hat{\theta}_\mu}{dt} = \gamma_\mu e_y S y \quad (13)$$

$$\frac{d\hat{\theta}_s}{dt} = \begin{cases} \gamma_s (\Gamma_1 D + \Gamma_2), \\ \text{if } \theta_s > \varepsilon_s \text{ or } \theta_s > \varepsilon_s \text{ and } (\Gamma_1 D + \Gamma_2) > 0 \\ 0, \text{ otherwise} \end{cases} \quad (14)$$

$$\frac{d\hat{\theta}_I}{dt} = \begin{cases} \gamma_I (\Gamma_3 D + \Gamma_4), \text{ if } \theta_I > \varepsilon_I \text{ or } \theta_I > \varepsilon_I \\ \text{and } (\Gamma_3 D + \Gamma_4) > 0 \\ 0, \text{ otherwise} \end{cases} \quad (15)$$

where,

$$\Gamma_1 = -\frac{e_y (1 - \hat{\theta}_I S^2) (S_i - S) y}{1 + \hat{\theta}_S S + \hat{\theta}_I S^2} \quad (16)$$

$$\Gamma_2 = \frac{e_y (1 - \hat{\theta}_I S^2) \theta_k y^2}{1 + \hat{\theta}_S S + \hat{\theta}_I S^2} - \frac{e_y \hat{\theta}_\mu S^2 y}{1 + \hat{\theta}_S S + \hat{\theta}_I S^2} \quad (17)$$

$$\Gamma_3 = -e_y S (S_i - S) y + \Gamma_1 \quad (18)$$

$$\Gamma_4 = e_y S \theta_k y^2 + S \Gamma_2 \quad (19)$$

and with the initial condition  $\hat{\theta}_s(0) \geq \varepsilon_s = \frac{1}{K_{S,\max}} > 0$ ,

and  $\hat{\theta}_I(0) \geq \varepsilon_I = \frac{1}{K_{S,\max} K_{I,\max}} > 0$ .

The update laws are projection algorithms that ensures that  $\hat{\theta}_s \geq \varepsilon_s > 0$  and  $\hat{\theta}_I \geq \varepsilon_I > 0$ .

By using appropriate mathematical arguments (that invoke in particular LaSalle invariance principle and Barbalat's lemma), it has been shown that if the dither signal fulfils some excitation persistence condition then the parameter estimates converges to their true values and the control error  $z_S$  converges to zero (Titica et al., 2003; Marcos et al., 2004).

## 5. SIMULATION RESULTS

The ED-TOC and the AES were tested using Matlab simulations, under different scenarios, for the same discontinuous reactor model. Each scenario in Table 2 provides a different challenge to the controllers.

The default kinetic model parameters and yield coefficients used to simulate the plant are:

$$\mu_0 = 0.53 h^{-1}, K_S = 1.2 g/L, K_I = 0.22 g/L \\ k_1 = 0.4, k_2 = 1.0$$

The initial states, unless otherwise explicitly said, used during numerical simulations are:

$$S_o = 2.0 g/L, X_o = 7.2 g/L, V_o = 1.0 L$$

and the substrate concentration in the inflow is  $S_i = 20 g/L$ .

The optimality parameter for the ED-TOC controller was set to  $P=0.98$  to calculate results in Table 3.

The design parameters for the AES controller were set to:

$$\gamma_\mu = 10, \gamma_s = 200, \gamma_I = 200, k_{y,0} = 20, k_z = 0.5, k_d = 1, \\ \varepsilon = 0.2. \text{ The dither signal } a(t) \text{ is chosen as:}$$

$$a = \sum_{i=1}^5 A_{1i} \sin[(0.001 + (5 - 0.001)i/4)t] + \sum_{i=1}^5 A_{2i} \cos[(0.001 + (5 - 0.001)i/4)t] \quad (20)$$

where  $A_{1i}$  and  $A_{2i}$  are normally distributed random numbers in the interval  $[-0.1, 0.1]$ . For details about the selection of the dither signal, the reader is referred to (Titica, et al., 2003).

The control objective is to fill the tank and obtain an amount of biomass, equal to that produced by the optimal trajectory, in the smallest possible time. The final reaction time  $t_f$  has been defined as the instant when  $V(t_f) = V_{max} = 40L$  and  $S_f = S(t_f) < 0.01$  g/L, where this last value has been arbitrarily assigned.

An optimality index is defined as  $t_{f_{opt}}/t_f$ , where  $t_{f_{opt}}$  is the optimal, theoretical minimal, finishing time. Table 2 presents the optimality index for each case. It shows that the performance of both controllers is good and close to 100%, except in Scenarios 2 and 6. In Scenario 2 bad initial conditions for the kinetic parameters are given and, additionally, in Scenario 6 a sudden change in plant's kinetics is produced. In both cases the AES performs in a less optimal way because it requires some convergence time to adapt the estimated values of the true parameters of the plant, and meanwhile the AES uses a non-optimal set point. As long as the total change in  $S^*$  is not big enough to cause big efficiency losses, the performance will not be greatly affected. This is the case if some history about the plant's behavior exists, so the initial conditions for every new batch can be given in a trustable fashion. By comparison, the performance effect in the ED-TOC is almost negligible, if any. This is so because its operational principle is of the bang-bang type, meaning that at every instant in time it will do the best possible action to get the system in the  $P$ -optimal zone, without the need for allowing

any parameter to converge. So the time the system spends away of the defined  $P$ -optimal zone depends only on the actuator limits and the plant dynamics. No equilibrium or set points are searched for. Its only aim is to keep the controlled variable inside the  $P$ -optimal zone during the singular arc. These are the main philosophical differences in both approaches. Table 3 shows another characteristics that define the main practical differences of the two controllers.

Some complementary differences between the two methods suggest some work should be done to combine them. In the AES, information about the plant is generated, as the values of the kinetic parameters are estimated in time. More sensors are used thus generating more data, specially  $S$  data. Other than the dither signal, it does not produce cycling of the input. On the other hand the ED-TOC is immune to tuning problems and model uncertainties (Table 3). It performs the bang-bang arcs in an exact way, same as the theoretical optimal solution. While doing the arcs it may know the  $t_k^*$  instants when  $S = S^*$  but does not know  $S(t_k^*)$ .

Figures 4 and 5 show the simulation results for Scenario 6. In Figure 4 it is clear that the dither in  $F$ , produced by the ED-TOC, is only plant-dependent, and that its convergence to new operation conditions is not governed by any controller's dynamics. The amplitude and time cycle of the bang-bang control signal depends only on the plant, and during the bang-bang arcs it operates perfectly. On the other hand, the AES graciously adjust its estimated value for the set-point of the manipulated variable (see dotted line in Figure 5), using an adaptive algorithm that requires a convergence time and that depends not only on the plants behavior in the new operational zone but also on the careful selection of the tuning parameters.

Table 2 : Optimality results for different scenarios for both controllers

Test Scenario for simulation comparison	Optimality index: $t_{f_{opt}}/t_f$ [%]	
	ED-TOC	AES
1. Default: $\mu_0 = 0.53$ $K_i = 0.22$ $K_s = 1.2$ ( $S^* = 0.5138$ ), True initial conditions given.	99.8	99.7
2. Bad initial kinetics given: $\mu_0 = 0.108$ $K_i = 1.645$ $K_s = 0.01$ ( $S^*$ decreased 50%)	99.8	89.5
3. Bad $S_0$ given (increased 50% respect to the real value)	99.8	99.7
4. Measurement error of +20% for $y$ in $t = (20, 30)$	99.8	99.8
5. Measurement error of +20% for $S$ in $t = (20, 30)$	99.8	99.8
6. $S_0 = S^*$ , bad initial conditions given ( $S^*$ increased 100%), and $S^*$ changed for $t = (20, 50)$ : $\mu_0 = 0.53$ $K_i = 0.44$ $K_s = 2.4$ ( $S^*$ increased 100%)	99.1	96.5

Table 3 : Characteristic differentiation of both control philosophies

Characteristics	ED-TOC	AES
Measured variables:	$y$ (used as $\gamma$ )	$S, y$
Controlled variables:	$\mu$	$S$
Manipulated variables:	$F$	$D$
Tuning parameters:	-	$\gamma_\mu, \gamma_S, \gamma_i, k_z, k_{y,0}, k_d, \varepsilon, a$
Optimality parameters:	$P$	-
Initial conditions required:	-	$S(0), y(0), S_f, \theta_\mu(0), \theta_S(0), \theta_i(0)$
Convergence speed depends on:	Plant and actuator limitations only	Plant and control tuning parameters
Control type:	Hybrid (Bang-bang + continuous)	Continuous

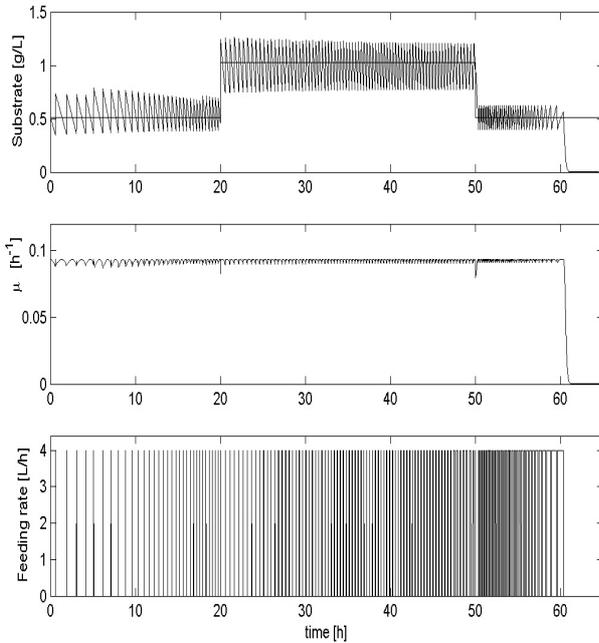


Figure 4: ED-TOC behavior using  $P=0.98$  for Scenario 6 in Table 2. In the substrate plot  $S^*$  is drawn with a step-like line.

## 6. CONCLUSIONS

Two control approaches of different philosophical nature have been compared, to understand their differences and complementarities, in a bioreactor example. The ED-TOC aims at keeping the system inside a predefined  $P$ -optimal zone. The AES aims at stabilizing the system in an optimal set point that is adapted on line. Both of them performed in a near optimal way for different test scenarios.

Advantages and disadvantages of the two philosophically different approaches were discussed, suggesting the possibility to combine them to obtain the better of each one of them. The idea is that while the system starts a batch, ED-TOC will perform in the best possible way for the singular arc. At the same time, if a  $S$  measure is available, during this bang-bang cycle a clear estimation of the  $P$ -optimal zone will be made in terms of  $S$ , including a measure for  $S^*$  at  $t_l^*$ . This value will be used to initialize the AES and, from then on, control could be made using AES policies. From time to time a bang-bang cycle could be run to test for optimality. This will reduce the on/off switching and at the same time bring valuable information about the plant model, and allow reacting to unforeseen perturbations or faults.

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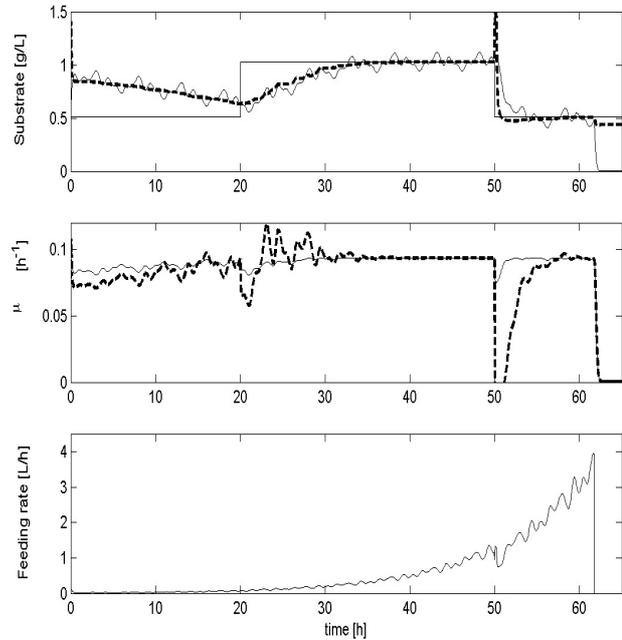


Figure 5: AES behavior for Scenario 6 in Table 2. In the substrate plot a step-like line shows  $S^*$ . Estimations are drawn with dashed lines.

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