CONTROL STRATEGIES FOR TREATING TOXIC WASTEWATER USING BIOREACTORS

Manuel J. BETANCUR^{1*V} Jaime A. MORENO¹ Iván MORENO-ANDRADE² Germán BUITRÓN²

 ¹Automation and ²Environmental Bioprocesses Departments, Institute of Engineering, National University of Mexico, UNAM, Ciudad Universitaria, CP 04510, Mexico DF.
 *Email: MBetancurB@iingen.unam.mx (+52) (55) 56233600 x 8816; fax 56228130
 ^{\[V]} on leave from Universidad Pontificia Bolivariana, UPB, IEO, A+D

Abstract: Different control strategies are compared, in regard to issues associated to biomass inhibition when treating toxic wastewater, to operate sequencing batch bioreactors. In particular the problem of time optimal operation and also the problem of handling sudden unknown toxicant peak concentrations are addressed. Because of the application characteristics it is not feasible, nowadays, to measure all of the important variables, thus little information is available online for controlling the process. One of the alternatives presented, the Event-Driven Time Optimal Control, offers to solve all problems, using only the practically available variables, even if uncertainties are present in the mathematical model of the bioreactor. *Copyright* © 2005 IFAC

Keywords: optimal control, software-sensor, fed-batch, bioreactor, toxic wastewater.

1. INTRODUCTION

Biological treatment of highly toxic wastewater, as such produced by the chemical and petrochemical industries, is a difficult task. Discontinuous sequencing batch reactors (SBR) have demonstrated their superiority for uses in wastewater treatment (WWT), compared to continuous reactors, mainly because of their performance. This paper shows how SBRs may be further enhanced with the use of suitable control strategies. In general traditional SBR processes exhibit 3 characteristics: periodical repetition of a defined phases sequence (filling, reaction, settling, draw and idle time) for each batch, dynamical behavior of biological and physical reactions in time and a preprogrammed duration of each phase according to the expected results, i.e. Fixed Timing Control (FTC). The first interesting SBR problem to solve is related to instrumentation limitations: it is not feasible, nowadays, to use toxicant substrate concentration (S) measurements. Then, for the FTC strategy, an expert chooses the timing based on the expected values for the toxicant substrate concentration in the inflow (S_i). However, if the given reaction time falls short, the SBR will not finish the substrate degradation and then toxicants will be discharged at the end of the batch.



Figure 1. Biomass specific growth rate $\mu(S)$

To be on the safe side, the reaction time is usually set larger than necessary. This wastes time and potentially causes a second problem: if all toxicant substrate is quickly treated the biomass starves while waiting for the next phase. Starvation may alter biomass necessary acclimation to such toxicant (Coello et al., 2003; Buitrón and Moreno 2002). A third related problem is the lack of processing time optimality, i.e. toxicant treatment in minimum time. A fourth problem is model uncertainty, especially in the S nonlinear relation to μ , the biomass growth rate (see Fig.1). As substrate degradation rate is directly related to μ , it follows that the maximum degradation rate is attained when $S=S^*$, as only at this point μ reaches its global maximum μ *. But FTC does not take this into account. Filling is performed at the highest possible flow rate, i.e. pure batch mode, regardless of S_i value. Hence the maximum S value inside the reactor (S_{Batch}) is a function of the unknown S_i only. As typically S_{Batch} is higher than S* then "inhibited" is the, undesirable, normal status for the SBR (see Fig. 1) in FTC mode. A fifth potential problem, even worse, appears if a sudden unknown toxicant peak is fed to the SBR. Here S_{Batch} may go to the killing zone, endangering the SBR, i.e. permanently damaging the biomass.

The simplest way to improve FTC is to detect the end of the reaction phase, without measuring S, by using the Dissolved Oxygen concentration $(\mathbf{0})$, which is easy and cheap to measure, in a similar way as proposed in (Sheppard and Cooper, 1990). That is what the Variable Timing Control (VTC in Table 1) (Buitrón et al., 2003) does. In the past, optimal control theory has been used to tackle some of the SBR problems allowing finding the best feeding policy, i.e. fed-batch mode (Smets et al., 2002; Sarkar and Modak, 2003; Moreno, 1999), but it is usually necessary to know perfectly the model of the plant and to measure its whole state. These conditions are very restrictive: a perfect model and parameter knowledge is very often unrealistic and, in WWT, it is either impossible or very expensive to measure all state variables. Such Time Optimal Control (TOC), when influent pump actuator limits are considered, consists of three arcs. Fig. 2(b2) depicts, for the SBR model in Eq. (1-4), the optimal trajectory projected in the Substrate-Volume plane (TP-SV): a bang-bang arc that fills the SBR until $S=S^*$, a singular arc that controls the feeding to maintain $S=S^*$ (this is the vertical path of the TP-SV, meaning *S* does not change even if volume level V increases), and a final bang-bang arc that waits until S decays below some final S_f . As S is not available, two strategies, close to that theoretical TOC are proposed: observer based time optimal control (OBTOC in Table 1) (Vargas et al., 2000) and event based time optimal control (EDTOC in Table 1) (Betancur et al., 2004a and 2004b). They both use **O** as the key control variable. Besides, EDTOC provides robustness against model uncertainties. Other known alternatives, to cope with parameter uncertainties, are: to use adaptive algorithms to identify the parameters and adapt accordingly the control strategy (Bastin and Dochain, 1990; Van Impe and Bastin, 1995; Van Impe, 1998) or to use Adaptive Extremum-Seeking strategies (Marcos *et al.*, 2004; Titica *et al.*, 2003) but again they both require, for the WWT case at hand, unavailable state measurements. Hence they are not considered here.

Table 1 lists the control strategies proposed to face the five SBR problems described when operated in FTC mode. This paper presents a comparison between these control strategies, considering the practical issues involved. Section 2 states the mathematical model of the SBR, Section 3 explains the control strategies to be compared, Section 4 summarizes the experiments performed and some conclusions close the paper.

Table 1. Comparison of the main problems tackled by

different SBR control strategies (treating toxicants)				
(FTC)	(VTC)	(OBTOC)	(EDTOC)	
Fixed	Variable	Observer Based	Event Driven	
Timing	Timing	Time Optimal	Time Optimal	
Control	Control	Control	Control	
None	Starvation	Starvation	Starvation	
(usual)	Instrument	Instrument	Instrument	
		Optimality	Optimality	
		Peaks	Peaks	
			Uncertainty	

2. SBR MODEL

Equations (1-4) approximate the SBR model for the Filling and Reaction phases. Settling and Draw phases are of no relevance to the problems at hand.

$$\frac{dX}{dt} = \mu X - \frac{Q}{V} X \tag{1}$$

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

$$\frac{dV}{dt} = Q \tag{3}$$

$$\frac{dO}{dt} = -(k_2\mu + b)X + K_1a(O_s - O) - \frac{Q}{V}O$$
(4)

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

States X(mgVSS/L), S(mg4CP/L), V(L) and O(mg/L)represent Biomass, Substrate, Volume level and Dissolved Oxygen concentrations respectively, S_i denotes the substrate concentration in the influent, k_1 and k_2 are yield coefficients, b is the endogenous respiration coefficient, Q(L/h) is the influent flow, the manipulated variable, $\mu(h^{-1})$ is the specific biomass growth rate, $\mu_o(h^{-1})$ is a parameter related to μ^* , K_S is known as the saturation constant and K_I as the inhibition constant.

3. CONTROL STRATEGIES

Fig. 2(a2) shows the SBR TP-SV when FTC is used. Note that the horizontal part of the TP-SV indicates there is no filling (V keeps constant). In this condition the toxic substrate concentration Sdiminish because of biomass action. To assure that Sgets below some final acceptable S_f before finishing the batch, some fixed time is allowed.

3.1. VTC (Variable Timing Control)

The variable timing control is similar to the FTC. Its TP-SV is exactly the same. The difference is that the reaction time is no longer fixed. Fig. 2(a1) shows a Near-End Detection (NED) module that signals the end of the reaction using the **O** dynamics expressed in Eq. (4), without the need to measure S. Note that after filling the SBR, for a given constant aeration rate, **O** will exhibit a unique minimum in time, closely related to the moment of maximum metabolic activity. Such maximum activity implies the maximum degradation rate and hence maximum **O** consumption. It happens just when $S=S^*$. When **O** rises again it is because activity decreases and **O** consumption diminishes, indicating the depletion of toxicant substrate. At this time the NED detects the end of the reaction and signals the sequencing module in Fig. 2(a1)) to proceed with the next phases to finish the batch.

3.2. OBTOC (Observer based time optimal control)

Observer based time optimal control is presented in Fig. 2(b1). Its ideal TP-SV is shown in Fig. 2(b2).

Note it is exactly the same as TOC's. If S could be measured and if all parameters were perfectly known, including S_i , it would be easy to implement the TOC. But that is not the case. Instead, OBTOC uses a *software-sensor* to estimate $\hat{S} \approx S$ by measuring O and V. Note that if OBTOC follows the ideal TP-SV it solves, simultaneously, some of the problems stated in the introduction. It delivers time-optimality without measuring S. It also prevents inhibition to occur when toxic peaks arise in the influent (at least for known S_i). As finishing time is known, starvation may also be prevented.

However there are various drawbacks related to the fact that this is a model based solution. The influent's substrate concentration (S_i , not easily measurable) needs to be known exactly. Also critical parameters need to be well known, as S^* for example. Even little mistakes in estimating these values affect the *software-sensor* performance, causing the actual TP-SV to diverge from the TOC one. For this reason the OBTOC solution is considered non robust and hence difficult to successfully apply in practice.



Figure 2. a) VTC, b) OBTOC, c) EDTOC; 1) Control Diagram, 2) Trajectory projection in S-V plane (TP-SV) Secondary axis is for μ or γ respectively. Initial conditions S=0 and $V=V_o$ are assumed. The dark area indicates the zone in which the process spends most of its reaction time.

3.3. EDTOC (Event driven time optimal control)

This method uses a different approach to cope with the lack of measurements and the uncertainties in model parameters while allowing to operate the SBR in a near optimal way. The strategy is based on the following observations. In the OBTOC case, for the non singular arcs, bang-bang control implementation was robust against uncertainties and information requirement was low. The problem was implementing the singular arc solution. Our proposal is then to replace the smooth and sensible singular signal with a bang-bang one that maintains its trajectory near and around the ideal singular trajectory. The generated error may be made, theoretically, as little as desired (Moreno, 1999). Robustness is linked to the well known properties of sliding mode control (Khalil, 2002; Slotine and Li, 1991). The low information requirement is related to the fact that only the singular surface needs to be estimated in the state space. Such surface is associated to certain events that depend on internal variables. If such events could be softwaresensed using the measurable variables, then a practical solution becomes feasible. Even more, if the singular surface is robustly related to such events, the solution will be robust against model uncertainties.

The EDTOC in Fig. 2(c1) does not measure S, but estimates a variable (denoted γ) related to the substrate degradation rate. Such γ could be estimated in real-time using O and V with Formula (6), which is easily obtained multiplying Eq. (4) by V and naming the total biomass as B=XV. Note that biomass growth is small during one bang-bang cycle, i.e. $B\approx$ constant.

$$\gamma = (k_2 \mu + b)B = K_1 a V (O_s - O) - QO - V \frac{dO}{dt}$$
(6)

Compare μ and γ in Fig. 2(b2) and Fig. 2(c2). They do have the same shape and both have a global maximum for $S=S^*$. But the advantage of having γ is that its maximum can be detected in real time, without knowing neither *S* nor *S*^{*}. That is why it is possible to manipulate the inflow Q in such a way that γ stays inside the "fast zone" of Fig. 2(c2). A similar zone exists for μ (not shown). Such a zone resides above P% of the maximum. The hatched rectangle in Fig. 2(c2) allows to explain how to maintain Soscillating between some S_{pl} (lower than S^*) and some S_{ph} (higher) all the way during the SBR filling. Each time S is about to leave such a range, an event is generated and then the EDTOC commutes Q (*on/off*) to prevent it. This explains the zigzag in the TP-SV. As $P \rightarrow 100\%$ the zigzag will be finer and then the control behavior will be closer to the TOC. This solution works regardless of the S_i value and regardless uncertainties and/or changes in most of the SBR parameters.

Only $K_l a$, as function of V(L) and airflow, and O_s , as function of $T(^{\circ}C)$, are required to estimate γ and it is not necessary to known them exactly. That makes the EDTOC robust. Even more, an error increment in parameter values will degrade EDTOC performance only gradually, that is, if parameter values are given far from real values, EDTOC will still behave acceptably. This reason makes such a solution a good candidate for practical use in industrial environments.



Figure 3. EDTOC finite state machine

Formally the EDTOC is represented by a finite state machine in Fig. 3, and the events that generate the state transitions are given in Table 2.

Table 2. EDTOC events for fed-batch processes

Event	Trigger	Estimates	Meaning
$e_{1.0}$	$d\gamma/dt > 0$	$S < S^*$	NonInhibited
$e_{2.0}$	$d\gamma/dt < 0$	$S > S^*$	Inhibited
$e_{2.1}$	$\gamma \leq P \gamma_{\kappa} *$	$S = S_{ph}$	Wait
$e_{1.2}$	$\gamma \leq P \gamma_{\kappa} *$	$S = S_{pl}$	Fill
e _{3.}	$V \ge V_{max}$	(measured)	TankFull
<i>e</i> _{4.}	$\gamma < \gamma_{end}$	$S < S_f$	ReactionEnd

Table 2 shows the events estimated by the eventdetector in Fig. 2(c1). Using such events the EDTOC commutes the influent pump Q. Initial state for k=0 at $t = t_0 = 0$ is always σ_0 . If inhibited, the system will instantaneously jump to state σ_2 . After the initial *bang-bang* arc, cycling between σ_1 and σ_2 will approximate the singular arc of the optimal solution. Once the tank gets full, σ_3 will complete the last *bang-bang* arc. Reaction will be ended when σ_4 is reached and, after that, the remaining of the batch phases will take place.

4. EXPERIMENTAL RESULTS

A laboratory 7L SBR with constant airflow (2 LPM) was used. Sludge from a municipal WWTP was acclimated to treat synthetic wastewater containing 4-chloro-phenol (4CP). The toxicant concentration for acclimation was S_i =350mg4CP/L. Applying twice such a concentration directly to the tank would inhibit and stress the biomass. Bigger concentrations in the tank may even permanently disable the SBR.

A series of experiments was performed to determine the effect of the various control strategies on different problems, especially peak toxicant concentrations tolerance and time optimality. Previous to each experiment the SBR was acclimated in FTC mode.

In all VTC, OBTOC and EDTOC experiments the end of the reaction phase was successfully detected, thus no accidental starvation was ever registered.

Different observer configurations were tested for implementing the OBTOC. The best results were obtained using an extended Kalman filter, so this is the one used for this experiment series. Results are presented in Figures 4 and 5. Figure 4 shows the toxicant removal efficiency $R=(S_i-S_f)/S_i$ when increasing toxicant input concentrations are applied. It can be seen that FTC and VTC strategies fail to remove all toxicant when its input concentration rises over 700mg4CP/L and the SBR gets practically disabled for concentrations over 1400mg4CP/L. OBTOC performs much better and keeps treating all the substrate up to concentrations of 1400mg4CP/L. For higher S_i the OBTOC failed to keep the substrate concentration inside the SBR's tank in the expected range, so the experiments were stopped. That means that over such concentration uncertainties render the OBTOC useless, even when special care was put to estimate the SBR parameters as exactly as possible. EDTOC performance was even better. Total removal was achieved for all experiments performed up to the maximum allowable range of 11200 mg4CP/L (it was not possible to dilute higher concentrations for the given nutrients and toxicants). In short, the falling lines in Fig. 4 indicate the toxicant input concentration that renders each control strategy to a condition in which the SBR gets inhibited and no longer performs appropriately the toxicant removal treatment.



Figure 4. SBR toxicant removal efficiency (R%), for various input toxicant concentrations, using various control strategies. No data yet available for EDTOC for S_i higher than 11200 mg4CP/L

Figure 5 gives an idea of the performance of the SBR operation. A comparison is made, for each control strategy, between the removal speed for the standard case and the removal speed when input toxicant peaks of increasing value are applied. It suggests that, in practice, for the experiments performed, EDTOC performs the best. In fact, independent measurements (not shown) confirm that at all times EDTOC maintained the substrate concentration S inside the SBR's tank at levels near the desirable S^* , even for large S_i input peaks.

Experiments show that EDTOC was capable to cope with input toxicant concentration peaks one order of magnitude higher than the ones tolerated by the strictly model based OBTOC, which in turn behaved in a superior way compared to FTC and VTC modes. As the EDTOC is also a simple and robust strategy, it seems reasonable to dedicate some additional lines and graphs to analyze in detail one of its experiments.



Figure 5. SBR relative efficiency (E%), for various toxicant concentration inputs, using various control strategies. The average degradation rate is compared to the acclimated condition.



concentration $S_i = 634 \text{mg4CP/L}$

Fig. 6 shows the results for an experiment to treat 4CP. EDTOC was used, implementing γ from Eq. (5). Toxic substrate concentration inside the reactor S (see 4CP in Fig. 6, square marks) was measured off-line, using manually taken samples. These values were not used with control purposes. Values up to S=200mg4CP/L are considered normal and safe for the biomass. An identification exercise later revealed $S^* = 13.99 \text{ mg4CP/L} \pm 7.4\%$ for a confidence interval of 95%. Fig. 6 shows that S was kept oscillating around S^* , in an acceptable concentration range. This was made by properly commuting on and off the influent's pump (Fig. 6, continuous thick line). Such behavior corroborates the effectiveness of the EDTOC strategy.

P=0.9 was chosen for all EDTOC experiments. Theoretically this implies a treatment time near to 5% higher than the optimal one.

Total biomass was B=1.4gVSS, exhibiting an increase of less than 2% for the whole reaction. Neither B, S, S_i nor S^* values were used by the controller.

 K_{la} was determined experimentally. Simulations were used to assess error tolerance to this parameter. Results show that errors in the range (-30%, +100%) are tolerable.

It must be noted that an additional perturbation is provided by the sensor used to measure the Dissolved Oxygen concentration (Fig. 6, thin continuous line). The sensor introduces some noise, and second order delays, to state variable O. This means that distortion and delays are to be expected when calculating γ from Eq. (5) (Fig. 6, dotted line) to use it in EDTOC. But, thanks to EDTOC robustness, the system did cope with all these perturbations and uncertainties.

5. CONCLUSIONS

From comparing different control strategies for toxic wastewater treatment (WWT) in sequencing batch reactors (SBR), and from experimental results, so far it is possible to draw some important conclusions:

Starvation at the end of a SBR batch cycle, an undesirable time period in which biomass lacks feeding that may happen when using the fixed timing control (FTC), could be avoided by applying either variable timing control (VTC), observer based time optimal control (OBTOC) or event based time optimal control (EDTOC).

Actual instrumentation limitations could be avoided if, instead of trying to measure Toxicant Substrate concentrations, Dissolved Oxygen concentration is measured, and then *software-sensor* are used to obtain the necessary information for control.

Uncertainties in the model and parameters affect the OBTOC, but are no problem for the EDTOC. The tradeoff is that EDTOC will always be sub-optimal even if the SBR model is perfectly known. In practice, however, EDTOC behaved better than OBTOC.

Input toxic concentration peaks are a problem for the FTC and VTC strategies. OBTOC can cope with peaks up to 1400mg4CP/L, while EDTOC behaves well for concentration one order of magnitude higher.

Strategies as the OBTOC and specially the EDTOC increase the performance of the SBR to levels never attained before. Research to further develop such operation modes is very promising. However, more experiments should be performed to finish this study. Long term biological stability should be addressed for the SBR when operated in Time Optimal Control (TOC) modes before categorically stating its benefits. This includes specially a study of the biological properties of the biomass when continuously subjected to this type of strategies.

ACKNOWLEDGEMENTS

Thanks to PAPIIT-UNAM (Project IN111905-2) for its financial support.

This paper includes results of the EOLI project that is supported by the INCO program of the European Community, Contract number ICA4-CT-2002-10012. M. J. Betancur thanks also UPB.

The scientific responsibility rests with the authors.

- Bastin, G. and D. Dochain (1990). On-line estimation and adaptive control of bioreactors. Elsevier.
- Betancur, M.J., J. Moreno and G. Buitrón (2004a). Event-driven control for treating toxicants in bioreactors. aerobic sequencing batch 9th International Symposium Computer on *Applications* Biotechnology in (CAB9). March 28-31, 2004. Nancy, France.
- Betancur, M.J., J. Moreno and G. Buitrón (2004b). Practical Optimal Control for Fed-Batch Bioreactors. *Preprints of NOLCOS 2004*, 1517-1522, Sep 01-03, 2004, Stuttgart, Germany
- Buitrón, G. and J. Moreno (2002). Modeling of the acclimation/deacclimation process of a mixed culture degrading 4-chlorophenol, Proc. 5th IWA Chemical Industry Group Conference, Nimes, France, 179-186.
- Buitrón, G., M. Schoeb and J. Moreno (2003). Automated sequencing batch bioreactor under extreme peaks of 4-chlorophenol. *Water Science* and Technology, 47(10), 175-181.
- Coello, M.D., J.A. López-Ramirez, D. Sales and J.M. Quiroga (2003). Evolution of an activated sludge system under starvation conditions. *Chem. Eng. Journal*, 94, 139-146.
- Khalil, H.K. (2002). Nonlinear Systems. 3rd. ed. Prentice Hall, Upper Saddle River, N.J.
- Marcos, N., M. Guay, D. Dochain and T. Zhang (2004). Adaptive Extremum-Seeking control of a continuous bioreactor. J. Proc. Control, 14(3), 317-328.
- Moreno, J. (1999). Optimal time control of bioreactors for the wastewater treatment. *Optimal Control Applications and Methods*, **20**, 145-164.
- Sarkar, D. and J.M. Modak (2003). Optimisation of fed-batch bioreactors using genetic algorithms. *Chemical Engineering Science*, 58, 2283-2296.
- Sheppard, J.D. and D.G. Cooper (1990). Development of computerized feedback control for continuous phasing of Bacillus subtilis. *Biotechnology and Bioengineering*, **36**, 539-545.
- Slotine, J.J. and W. Li (1991). Applied nonlinear control. Prentice Hall, Englewood Cliffs, N.J.
- Smets, I.Y.M, K.J.E. Versyck and J.F.M. Van Impe (2002). Optimal control theory: a generic tool for identification and control of (bio-)chemical reactors. *Annual Reviews in Control*, 26, 57-73
- Titica, M., D. Dochain and M. Guay (2003). Adaptive Extremum-Seeking Control of Fed-Batch Bioreactors, *European J. of Control*, 9, 614-627
- Van Impe, J.F.M. (1998). Optimal control of fed-batch fermentation processes. In: Advanced Instrumentation, Data Interpretation, and Control of Biotechnological Processes (J. Van Impe, P. Vanrolleghem and D. Iserentant, Eds.). pp 319-346. Kluwer Acad. Pub. Dordrecht-Boston-London.
- Van Impe, J.F.M. and G. Bastin (1995). Optimal adaptive control of fed-batch fermentation processes. *Control Eng. Pract.*, **3**(7), 939-954
- Vargas, A., G. Soto, J. Moreno and G. Buitrón (2000). Observer based time-optimal control of an aerobic SBR for chemical and petrochemical wastewater treatment. *Water Science and Technology*, **42** No. 5-6, 163-170.