EVENT-DRIVEN TIME-OPTIMAL CONTROL FOR A CLASS OF DISCONTINUOUS BIOREACTORS

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Keywords: fed-batch, time optimal control, software sensor, discontinuous bioreactor, SBR

Short Running Title:

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SUMMARY

Discontinuous bioreactors may be further optimized for processing inhibitory substrates using a convenient fed-batch mode. To do so the filling rate must be controlled in such a way as to push the reaction rate to its maximum value, by increasing the substrate concentration just up to the point where inhibition begins. However, an exact optimal controller requires measuring several variables (*e.g.* substrate concentrations in the feed and in the tank) and also good model knowledge (*e.g.* yield and kinetic parameters), requirements rarely satisfied in real applications. An environmentally important case, that exemplifies all these handicaps, is toxicant wastewater treatment. There the lack of online practical pollutant sensors may allow unforeseen high shock loads to be fed to the bioreactor, causing biomass inhibition that slows down the treatment process and, in extreme cases, even renders the biological process useless. In this work an *Event-Driven Time-Optimal Control* (ED-TOC) is proposed to circumvent these limitations. We show how to detect a "*there is inhibition*" event by using some computable function of the available measurements. This event drives the ED-TOC to stop the filling. Later, by detecting the symmetric event, "*there is no inhibition*", the ED-TOC may restart the filling. A fill-react cycling then maintains the process safely hovering near its maximum possible reaction rate, allowing a robust and practically time-optimal operation of the bioreactor.

Two application study-cases are presented: one including experimental results, a wastewater treatment process where the dissolved oxygen concentration is used to detect the events; the second is a biomass production process simulation, where a gaseous product measurement is used instead.

INTRODUCTION

Many important industrial cyclical processes are carried out using discontinuous bioreactors *e.g.* antibiotics and enzymes production, biomass production (*e.g.* baker's yeast), or even wastewater treatment. When an inhibitory substrate is fed, using the simple batch strategy with an open-loop *Fixed Time Control* (FTC) will not be optimal for their operation. This is so mainly because the (fast) filling phase increases the substrate concentration, in the tank, to levels that cause biomass inhibition, lasting during most of the reaction phase. There is experimental evidence that the inhibitory peak of substrate, accumulated during the feeding, may be reduced just by increasing the filling time (Tomei *et al.,* 2003). However, any feeding policy that allows a continuous substrate accumulation inside the reactor will produce inhibition, which in turn contributes to speed up such accumulation, which augments inhibition, and so on. This *snowball effect* was described by Chang (2003), along with a fed-batch control proposal to avoid it by properly manipulating the feeding rate. One key result, obtained from studying the structure of the mathematical model of this class of processes, is that, in many cases, the final product yield can be maximized simply by maximizing the instantaneous yield (Modak *et al.*, 1986). This result may be used also to design a *Time Optimal Control* (TOC), to manipulate the feed flow rate in order to maintain a substrate concentration that maximizes such an instantaneous yield (Moreno, 1999; Sarkar and Modak, 2003; Smets *et al.*, 2002). But, to implement the TOC avoiding the snowball effect trap, it is usually required to know perfectly the mathematical model (*i.e.* both structure and parameters) of the process and to measure all important process variables *i.e*. all concentrations, liquid level and inflow. In many applications these two conditions are very restrictive: perfect model knowledge is very often unrealistic and, in biotechnology and wastewater treatment, it is either impossible or very expensive to measure all variables. In order to cope with the first problem different robust approaches have been proposed in the literature. Most often adaptive algorithms identify the parameters of the (otherwise assumed well known) model, and adapt accordingly the control strategy (Bastin and Dochain, 1990; Van Impe, 1998; Van Impe and Bastin, 1995). Adaptive Extremum-Seeking strategies have been also proposed (Marcos *et al.*, 2004; Titica *et al.*, 2003), but they require substrate concentration measurements in order to asymptotically search for an optimal steady state. The measurement problem has been addressed mainly by using Software-Sensors *e.g.* Vargas *et al*. (2000) used the Dissolved Oxygen (DO) to estimate the substrate concentration for a WW case.

In this work a different approach to deal with the lack of measurements and with model related uncertainties, while practically optimizing process operation time, will be proposed. The main idea is based on the following observations. The exact TOC, when a realistic bounded inlet flow is considered, is composed of two bang-bang arcs (switching to maximum or to zero feed rate) and one, intermediate, singular arc (regulated inflow). 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 related uncertainties. More problematic is the determination and implementation of the singular arc. As the time horizon in a batch process is finite, asymptotic approaches are not always convenient. An exact solution, on the other hand, requires a good knowledge of the model and parameters, resulting thus sensitive, *i.e.* non robust, to uncertainties. The strategy we propose, an *Event-Driven TOC* (ED-TOC), replaces the exact, sensitive, and smooth singular control arc by a bang-bang one that maintains the process trajectory hovering around the singular surface. The additional reaction time spent by such a hovering can (theoretically) be made as small as desired (Hermes and LaSalle, 1969; Moreno, 1999). The advantage of this replacement is that it is very robust against uncertainties and, for its implantation, only a reduced quantity of information is required (Moreno, 1999). The requirement of low quantity of information is related to the fact that not all information about the system is really required. It is only necessary to determine the precise instants in time, at which certain specific events do happen, to decide when to switch ON or OFF the feed, *i.e.* the manipulated control variable. Such events are associated to internal variables but, for the considered class of processes, they could be software-sensed using just the measurable ones. Then it is feasible to implement a practical controller for the inlet flow, driven by such events, whose performance approximates the TOC one.

To illustrate the proposal, two study-cases are presented: one including experimental results, a wastewater treatment case where the Oxygen Mass Uptake Rate (OMUR), computed via online dissolved oxygen concentration measurements, is used for the events detection; and the other is a biomass production case, where the gaseous product production rate is used to detect the events.

MATERIALS AND METHODS

Toxic Wastewater (WW) Treatment case

For the lab experiments an automated aerobic discontinuous reactor with a capacity of 7L, with a 57% exchange volume, was used. The airflow rate was 1.5 L/min and the temperature was maintained at 20±1ºC inside the tank. Synthetic WW containing 4-chlorophenol (4CP) was used as the sole source of carbon and energy. Nutrients were added as recommended by AFNOR (1985). Volatile suspended solids (VSS) analyses were done according to Standard Methods (APHA, 1992), and then used to calculate the biomass concentration (X). The reactor was inoculated, and acclimated, with microorganisms from a municipal activated sludge WW treatment plant (B_0=14 gVSS) using the method described by Moreno-Andrade and Buitrón (2004). The substrate concentration (S) was reported offline, from manually taken samples, using a modification of the colorimetric technique of the 4-aminoantipyrine method (APHA, 1992). As a standard condition the reactor was operated cyclically using an influent concentration (S_i) of S_{std} (0.35 g4CP/L) and the next phase sequence: fill and react (204 min for the FTC and self-controlled for the ED-TOC), settle (30 min) and draw (6 min).

The ED-TOC was coded in *LabView,* from National Instruments (NI). NI hardware *PCI6025E* was used to interface the PC to the reactor. The DO was measured with a *COS4* Endress+Hauser sensor, and the feed rate (Q) was controlled with a Cole-Palmer *7523 Masterflex* pump. Only Volume level (V) and DO concentration (O) were used for online control purposes. In addition to the standard condition the ED-TOC was used to treat shock loads of increasing magnitude: S_i =(2, 8, 14, 20)S_{std}.

Biomass Production (BP) case

Simulations were performed, using a *MATLAB* environment, for a single BP case. Model parameters were chosen, the same as in Titica *et al.* (2003), to represent a realistic, inhibitory, Haldane law:

$$\mu_0 = 0.53\,h^{-1}, K_S = 1.2\,g/L, K_I = 0.22\,g/L, k_1 = 0.4, k_2 = 1.0, S_i = 20\,g/L$$

$$S_o = 2.0g/L, S_f = 0.01g/L, X_o = 7.2g/L, V_o = 1.0L, V_f = 40L$$

For the TOC simulation all variables are supposed to be perfectly measurable and all model parameters perfectly known. For the ED-TOC, instead, all parameter values are assumed unknown (*i.e.* they are unavailable for the controller) and only the gaseous production rate and V are measured.

THEORETICAL ASPECTS

In this section the mathematical model and the typical FTC operating strategy for the microbial growth process in a discontinuous reactor will be explained first. Then the time optimization problem will be considered, introducing the theoretical (exact) TOC law. Finally, the newly proposed ED-TOC strategy will be presented as a practical and robust alternative to implement the TOC.

Process Model for the Class of Bioreactors to be Time-Optimized

A Sequencing Batch Reactor (SBR) process consists of *phases*: fill, react, settle, draw, and idle (Wilderer *et al*., 2001). These may be independent (as in batch mode) or concurrent (as in fed-batch). They may even repeat. Such is the case in our proposal (…fill-react-fill-react…), which is somewhere in between batch and fed-batch. The following dynamical model (Smets *et al.,* 2002) explains the concurrence of the fill and react phases (for biomass and substrate concentrations, and volume level):

Equation (1) $$\frac{dX}{dt} = \mu X - \frac{Q}{V} X$$

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

Equation (3) $$\frac{dV}{dt} = Q$$

Let us call the model *nominal* when it represents the real plant, *i.e.* every parameter and variable are perfectly known, and *practical* when it represents the available information the controller has about the real plant, *i.e.* uncertainty is included in parameter, measurement and estimation values.

The difficulties for treating inhibitory substrates are related to the non monotonic behavior of the Biomass Specific Growth Rate (μ), which is proportionally related to the substrate reaction rate in Equation (2). Note, from Fig. 1, that if the substrate concentration S is kept well below S^* (the S value at which μ reaches its maximum value μ^*) there is no inhibition but the reaction is slow. If S is raised near S^* then the reaction is fast and yet safe *i.e.* the biomass is not affected by inhibition. If S surpasses S^*, then the reaction gets slow again, because of biomass inhibition. Now, if S is accidentally pushed much further up, inhibition effect builds up dangerously and the SBR may even get disabled.

Once the SBR is full, the reacting phase could be ended, practically, when the substrate concentration left in the tank decreases below some acceptable threshold S_f. For control purposes such a finishing criterion is useful even for different SBR applications. For example, in a single BP process this criterion means that the amount of substrate left to be converted into biomass is negligible *i.e.* the biomass already produced is acceptably close to the maximum possible one (obtainable only if an infinite reaction time is allowed). For a WW application the same criterion means that the toxic left inside the SBR is negligible, *e.g.* complies with the limits imposed by law, and settling may start.

Fixed Time Control (FTC)

This typical control mode uses no instrumentation to asses the terminal status, so there is no way to automatically finish the reacting phase. That is why a fixed reaction allowance time, large enough to tolerate perturbations, *e.g.* influent substrate concentration deviations from the standard condition, is usually set. The SBR gets filled from its residual volume level V_0, until full at V_f, using the maximum pump capacity Q_x. Hence S is typically quickly raised into the inhibition zone (Fig. 2A) to some S_{batch} value that depends on S_i. If it is too high there exists the risk to enter the stress zone (Fig. 1). That is why with FTC the biomass starts processing the substrate slowly and keeps doing so most of the reacting time, with no regard for time optimality. In applications such as WW treatment the advantage is that there is no need for costly and/or delicate instrumentation. But, because there is no feedback, there is always the risk that when a shock load (*i.e.* an unusually high substrate concentration) is fed to the SBR then the biomass gets too inhibited, and a yet polluted effluent will be drawn because the reaction will not have enough time to complete. Usually then the expert sets the reaction time larger than needed in order to prevent for such disturbances. But even then, if the perturbing shock is too high, the biomass may loose viability permanently (Buitrón *et al*., 2003). As a result the FTC mode, although apparently easy and economical to setup and to operate, provides neither optimization nor robustness for the process.

Time-Optimal Control (TOC)

In order to profit the most from a SBR it is desirable to increase the amount of batches that can be safely processed per time-unit *i.e.* to reduce each individual batch processing time. Let us call *TOC* any control strategy that manipulates the inlet flow in order to process a single batch in the minimum possible time. Note that, as settling and drawing phase's duration do not depend on the filling policy used, they cannot contribute to such an optimization. That is why only filling and reacting phases are to be considered, from now on, for studying the TOC.

Assumption 1: this study considers inhibitory models such that $\mu(S)\geq 0$ does have a unique maximum $\mu^*=(S^*)$ for $S\geq 0$ *i.e.* it should grow monotonically from $S=0$ to $S=S^*>0$ and then decrease, also monotonically, for $S>S^*$ (*e.g.* Fig. 1). Note that non inhibitory models may also be covered as the limit case when $S^*\rightarrow\infty$

The TOC combines the filling and reaction phases in a fed-batch mode. It fills the SBR gradually, not all at once, using the model knowledge to compute the best filling policy. If $S_0< S^*$ then the controller starts to fill at the highest possible rate (see long fat arrow in Fig. 2B and the resulting trajectory, projected in the Substrate-Volume *(SV)* plane, in Fig. 3A) but then, once S^* is reached, the first bang-bang arc ends and the control slows down the filling to an exact inflow rate $Q=Q_{opt}$, that provides just the exact amount of substrate needed to replace the consumed one, so that $S=S^*$ (see fed-batch point in Fig. 2B and fed-batch trajectory in Fig. 3A). Optimality requires completing exactly such a singular arc until the reactor gets full (Moreno, 1999) and then turning off the feed to perform the last bang-bang arc. Other initial case may arise if $S_0>S^*$. Then the filling should not start until the biomass naturally consumes the substrate down to the critical S^* value (see dotted trajectory in Fig. 3B).

Practical Optimality and Robustness

Let us define a *practically optimal,* or *robust,* zone (Fig. 4 and Fig. 5) by $\mu\geq p\mu^*$ with $0<p\leq 1$. Any controller that produces the bang-bang arcs exactly, and the singular one as an approximation living in such a zone, is said to be *practically optimal.* Practical optimality means that the time it takes the

reaction to finish (t_f), is close to the optimum one ($t_{f.opt}$) bounded by $t_f \leq t_{f.opt}+T_p$ where $T_p(p)\geq 0$ is a continuous function of p such that $T_p(1)=0$. If a controller remains being practically optimal in the presence of bounded errors, uncertainties, perturbations, or noise, it is said to be also *robust.*

TOC Practical Implementation Limitations

Implementations of the TOC strategy confront practical limitations, *e.g.* to calculate Q_{opt} accurately, that prevent them from being reasonably robust. For example, in the WW case, the key limitation is the unavailability of substrate sensors. Solutions have been proposed to estimate its concentration by using DO based software-sensors (Vargas *et al*., 2000). The main problem with such an approach is that the SBR model that links the DO to the substrate concentration is full of parameters that are either difficult to measure or uncertain (Buitrón *et al.*, 2005). Even more, parameters S^* and S_i need to be precisely known. This renders that type of solution non robust and difficult to apply industrially.

Event-Driven Time-Optimal Control (ED-TOC)

The ED-TOC may be considered as an approximation of the exact TOC, with the advantage that its realization avoids most implementation problems. The concept of *events*, their definition in terms of model parameters and of direct measurements of S and V, and how to use them for driving a robust *near-optimal* control will be explained in this subsection. The next one will explain how to use an *Events-Software-Sensor* (ESS) in order to avoid measuring S and to eliminate parameter dependency.

Assumption 2: the SBR is *optimizable i.e.* although the inlet flow is bounded by $0\leq Q\leq Q_{max}$, making $Q=Q_{max}$ always pushes S to increase, and allows it to overshot the robust zone ($S>S_{max}$) for some Volume level value in $V_0<V<V_f$.

The ideal objective of the ED-TOC, for an optimizable SBR (Assumption 2), may be redefined as to use ON/OFF inlet flow pulses to maintain μ value above some threshold $P\mu^*$, where $P\in(p,1]$ is a user defined parameter that allows to choose a *near-optimal* zone $S_{low}\leq S\leq S_{high}$ (Fig. 4) inside the robust zone. This definition leads the ED-TOC to naturally perform the initial and final bang-bang arcs of the TOC exactly, and to approximate the singular arc by a *zigzag* arc, also bang-bang, inside the near-optimal zone. If we choose $P \rightarrow 1$ then $S_{low}, S_{high} \rightarrow S^*$ (Fig. 5) and the zigzag arc (Fig. 4) will resemble TOC's singular arc (vertical line, Fig. 3A). The drawback is that inlet pump switching frequency augments when P does, so its value must be chosen considering such a practical constraint.

Events and Logical States for the ED-TOC

In this study an *event* (e), to drive the ED-TOC, is defined as a time dependant variable of the Boolean type (*i.e.* it is binary: 1=*true*=*the event is happening*; 0=*false*=*the event is not happening*). Events are the cues for *transitions i.e.* for changing from one logical *state* (σ) to another one in the *finite states machine* representation of the ED-TOC in Fig. 6. There, each circle represents a given state that the ED-TOC may take, one and only one, at any given time. Table I describes the meanings and control actions of all possible ED-TOC states during the filling and reacting phases. For example state σ_1, tagged as "fill", is described as the state when the inflow pump is ON and the ED-TOC is waiting for inhibition to be detected (e_1) or for the tank to get full (e_3). The occurrence of a given event, represented by arrows in Fig. 6, triggers a transition to a different state, the one pointed out by the respective event arrow. Table I presents a list of logical states and the events that force transitions between them. As example, σ_1 will be left only when events e_1 or e_3 occur. If e_1 occurs first the ED-TOC will jump to state σ_2 or, respectively, if e_3 to σ_3. Table II describes the relevant process events, the ones whose physical meaning is related to the process crossing of some switching surface.

The initial state σ_0, the one with an extra ring in Fig. 6, starts the filling ($Q=Q_{max}$) assuming the system is not inhibited. If such assumption is corroborated, by e_0 occurrence, then the ED-TOC jumps to σ_1 in order to finish performing the first arc of the TOC *i.e.* to initially fill the reactor as quickly as possible. But if e_5 occurs instead of e_0 this means the assumption is false and the initial conditions are not as expected. In that case the system jumps to σ_2 turning OFF the influent pump and waiting for the inhibition to disappear before continuing the filling *i.e.* until e_2 occurs. Whatever the initial condition was, once the system reaches either σ_1 or σ_2, a cycle begins in which both states alternate recursively, generating the zigzag *i.e.* the bang-bang approximation of the singular arc. Such a cycle is interrupted when e_3 occurs *i.e.* the tank is full. At this point the last arc is performed by σ_3. The reaction ends when e_4, the finalization criterion, is met. Then the settling phase should follow (not shown).

Note that, if $\mu(S)$ is known and if S is measurable, implementing the ED-TOC is easy: by choosing P the thresholds S_{low} and S_{high} may be straightforwardly obtained from $\mu(S)$. Then comparators would use the available S measurement to detect the events in Table II needed to drive the ED-TOC.

Event Errors and Practical Optimality

It should be noticed that for the ED-TOC the important feature in an event is its *occurrence, i.e.* the moment in time when the *false* to *true* transition takes place, as such is the instant when a state transition may be commanded. Hence an *event error* is defined as the time difference between the event occurrence in the nominal model and the practical one. Errors are expected in practical situations as it is normal to have uncertainty in practical model parameters and perturbations and/or noise in measurements. Now let us study the possible error types. Some remarks and definitions, related to Fig. 4, are in order before proceeding. Let us define a *segment* as a piece of the ED-TOC trajectory that is produced between state transitions, and let us call *zigzag* to the concatenation of at least two segments due to the cycling between states σ_1 and σ_2. Note that the zigzag is the only part of the trajectory susceptible of being significantly altered by errors. A trajectory is said to *hover* if all zigzag segments touch the near-optimal zone, and to be *practically-optimal* or *near-optimal* if all zigzag segments end inside the robust or near-optimal zone, respectively. A controller is said to be *hovering* if it produces trajectories that hover. Let us define T_E as the *escape time*, *i.e.* the minimum time it will take some segment originating in the near-optimal frontier to escape the robust zone, and T_R as the *returning time i.e.* the maximum time it will take some approaching segment, originated in the robust zone, to enter the near-optimal one. Let t_k be the time at which the k^{th} state transition should be produced in the nominal model and $\underline{t}_k$ the practical one. Then, the time it should take the k^{th} segment to be completed is $T_k=t_k-\underline{t}_{k-1}$. But if an event error happens during the k^{th} transition such a lapse will vary. Let us denote such a variation $E_k=\underline{t}_k-t_k$ as the *error value*. An error is said to be of the *delaying* type if positive (*bounded* if $E_k < T_E$) and of the *anticipatory* type if negative (*bounded* if $E_k > T_R - T_k$). It is *isolated* if $E_{k-1}=E_{k+1}=0$, and consecutive or *concatenated* otherwise.

Robustness in the presence of Event Errors

Let us now use the ideal ED-TOC trajectory in Fig. 4 to analyze errors impact. Such a nominal trajectory is near-optimal and error-free. Now assume an isolated delaying error occurs when a zigzag segment is ending *i.e.* just when touching the near-optimal frontier. Then, such a nominal segment will definitely be enlarged and it will grow out of the near-optimal zone. A sufficient condition to guarantee that the considered segment will not escape also the robust zone is that the perturbing error is bounded. On the contrary, if the error is anticipative, the segment will be shortened and it will stay in the near-optimal zone. If another zigzag segment follows, error isolation guarantees that it will not be subjected to an additional error, so it will necessarily search to touch the near-optimal zone frontier. In fact such a touching will be guaranteed even if there is a new (concatenated) error, as long as such an error is of the delaying type. But if the new error is of the anticipative type, and the previous segment ended outside the near-optimal zone, there is no guarantee that the new approaching segment will hover, unless it originates still inside the robust zone and lasts more than the returning time *i.e.* if the error is bounded. Using the previous analysis, it follows that the ED-TOC guarantees to be:

- Hovering for isolated errors of any type or for concatenated errors of the same type.
- Hovering for concatenations where every anticipatory error following a delaying one is bounded.
- Practically Optimal and Robust against (not necessarily bounded) anticipatory concatenated errors.
- Practically Optimal and Robust against any sequence of concatenated bounded errors.

Summarizing, the basic ED-TOC is near-optimal. It is also robust against most errors that might be produced by perturbations or uncertainties in model structure and parameters. Little information is needed about the inhibitory function or about most of the model parameters as long as Assumption 1 and Assumption 2 are satisfied. Another advantage is that a simpler, and less expensive, ON/OFF inlet pump may be used instead of a regulated one, as would be required to implement an exact TOC.

Let us consider an example illustrating uncertainty effects. Suppose, in Fig. 4, that the identified $\underline{S}_{low}$ is underestimated but still lies in $S_{min}<\underline{S}_{low}<S_{low}$. If everything else is perfect then the ED-TOC will produce a zigzag that is enlarged to the left and into the robust zone *i.e.* the errors are of the bounded delaying type and the trajectory is no longer near-optimal, but robustness holds. If $\underline{S}_{low}<S_{min}$ then error bounding disappears and robustness with it, although hovering still holds.

Events-Software-Sensor (ESS) based ED-TOC

If S is not measurable, or if μ is an uncertain function, then the basic ED-TOC explained earlier is not usable as it is. Let us now explain how to perform events estimation, indirectly, using an ESS. To *estimate* an event is to use related variables and indirect software-based methods to detect the instant in time at which the real event is supposed to be happening. To simplify the explanation in this section it will be assumed that $\mu_t(t)=\mu(S(t))$ is measurable and serves as the $\gamma(t)$ input to the ESS module (Fig. 7A). Later we will remove such an assumption. In Table II there is a column labeled *ESS function*. Such a function is used to estimate the events occurrence. This means that instead of measuring directly the (unavailable) S variable needed to evaluate some events occurrences, an indirect variable is used to estimate such transition instants. In the case at hand such a variable is chosen as $\gamma=\mu_t$.

Estimation of the unknown maximum μ^*

Note, in Table II, that for estimating e_1 and e_2 it is now necessary to use the unknown maximum $\gamma^*=\mu_t^*=\mu^*$ (please remember to use $\gamma=\mu_t$). Thus it is necessary to estimate also such a maximum value by using only the available measurements. We propose to use Equation (4) to perform the estimation (the underlined variable includes the estimation error while converging to the nominal value).

Equation (4) $$\underline{\mu}^* = \max_{\tau\in[0,t]} \mu_t(\tau)$$

It may be implemented by memorizing, in real-time, the maximum encountered value of μ_t. Note that the estimated value will converge to the true value as soon as μ_t reaches its maximum.

Estimation of the events

Let us analyze the procedure to estimate all of the events in Table II:

- Events e_0 and e_5: the filling phase begins when σ_0 is activated. Up to this point there is yet no trustable estimation available about μ^*, but this lack of information poses no problem as only events e_0 or e_5 are required to jump out of σ_0 (Fig. 6) and neither of them use it. As σ_0 commands the inlet pump ON (full flow) then S will increase because of Assumption 2. From Assumption 1 it follows that if increasing S causes μ_t to increase then $S<S^*$ (there is no inhibition) and e_0 is true. On the contrary, if μ_t happens to decrease, this means that there is inhibition and e_5 should be triggered instead of e_0. If there is no change in μ_t then σ_0 just holds until there is.
- Event e_1: this event is required only by σ_1 and such a state activates the inlet pump, making S increase. Initially $S<S^*$ so μ_t will keep increasing until it reaches μ^* and, meanwhile, e_1 will not trigger because ($d\mu_t/dt>0$). So far there is no need to know μ^* value. But once μ_t begins to decrease μ^* true value must be known in order to evaluate the inequality ($\mu_t \leq \mu^*$). However by that time μ_t derivative sign has changed meaning its maximum has been already reached, and so it was possible for Equation (4) to converge to a valid μ^* estimation and so the inequality value is sound.
- Event e_2: explanation is similar as for e_1
- Event e_3: this event detects when the SBR tank is full. No software-sensor is used. The volume level measurement V is directly compared to the desired final volume level V_f.
- Event e_4: A user defined parameter sets the $\mu_f=R\mu^*$ value at which the substrate that still remains inside the reactor is considered to be negligible.

Extended ED-TOC

In this subsection we show how it may be possible to implement the ED-TOC using just practically available measurements. Note that the ESS defined in Table II (Fig. 7A) uses only derivative signs and relations of γ to its own maximum. Then if a function that keeps the same derivative signs and relations as μ_t is used, the events are still going to be detected with no error at all. As example consider $\gamma=a\mu_t$. Even if the positive constant a is unknown, the ESS estimations will still be exact. This means that the ESS is robust against such a parameter, because it only needs for it to be positive, not its actual value. In general robustness, for any given Q, will hold, for some P, for any uncertain but well behaved $\gamma = f(\mu_t)$ *i.e.* any monotonic, continuous, positive and time-invariant function. But in practical applications, *e.g.* the ones considered in the study-cases, the easier and cheaper functions to measure and to compute are time-varying function of the type $f(\mu_t, t) = a\mu_t B(t)$, where a is a positive constant, but the multiplicative perturbation $B=XV$ (the total biomass) is not a constant but a positive increasing time-function. Let us analyze conceptually its practical effects and find sufficient conditions for keeping robustness when such a function type is used. From Equation (1) it is clear that biomass growth behavior is exponentially bounded by μ^*. Then Equation (5) represents an upper bound that can be used into the ESS as the worst case perturbation scenario.

Equation (5) $$\varphi = a\mu_t B_0 e^{\mu^* t}$$

Zigzag perturbations due to the ESS may be linked only to e_1 and e_2 being the terminal events of segments produced by σ_2 and σ_1 respectively. So the Q equality in Table II is always satisfied for both events, and their respective γ dependant inequalities are identical. Then the kind of error that might arise for both cases is the same, and may be studied by using the inequalities $\varphi \leq P\varphi^*$ and $d\varphi/dt \leq 0$, where φ^* is the previous local maximum of φ. Note that for using φ successfully in the ESS it must mimic μ_t behavior *i.e.* during any given zigzag segment φ should first grow to reach some maximum φ^*, and then decrease to match $P\varphi^*$. Otherwise the generated delaying error is infinite, thus not bounded *i.e.* the ED-TOC will not be robust. This suggests that the changes due to B should be small compared to changes in μ_t. Let us assume for now that this is the case and analyze any given k^{th} segment of the zigzag. It began at t_{k-1} and should end at t_k. Meanwhile μ^* was reached, in between, at some $t_{k-1} < t_\mu^* < t_k$. However, at this point, φ derivative in Equation (6) is positive *i.e.* φ is still growing, so its maximum $\varphi^* = \varphi(t_\varphi^*) > \varphi(t_\mu^*)$ will be reached only later, at $t_\varphi^* > t_\mu^*$.

Equation (6) $$\frac{d\varphi}{dt} = aB_0 e^{\mu^* t}\left(\frac{d\mu_t}{dt} + \mu_t \mu^*\right)$$

Now let us choose P=1 *i.e.* to define the near-optimal zone as a line. Under such settings the mistaken event is going to occur just when φ reaches its maximum, *i.e.* after μ_t has reached its own, so the produced error is necessarily of the delaying type (always). This condition is defined by Equation (7).

Equation (7) $$\frac{d\varphi}{dt} = 0 \quad \leftrightarrow \quad -\frac{d\mu_t}{dt} = \mu_t \mu^*$$

If it is not satisfied then $E_k \rightarrow \infty$, but such an error could be made bounded if we choose $T_E \geq t_\varphi^* - t_\mu^*$. This happens if the detection occurs before the segment leaves the robust zone. The inequality in Equation (8) results from expressing such a bounding in Equation (7) and represents a sufficient design criterion to guarantee robustness. Let us use Equation (2) to obtain Equation (9) and compare it to the robustness condition in Equation (8).

Equation (8) $$\mu_t(t_\varphi^*) \geq p\mu^* \quad \rightarrow \quad -\left.\frac{d\mu_t}{dt}\right|_{t_\varphi^*} \leq p\mu^{*2}$$

Equation (9) $$\frac{d\mu_t}{dt} = \frac{d\mu}{dS}\frac{dS}{dt} = \frac{d\mu}{dS}\left(\frac{Q}{V}(S_i - S) - k_1\mu X\right)$$

If the segment under consideration is produced by σ_2 then Q=0. As μ and k_1 are given by the biomass-substrate combination they may not be modified by the designer, but X may. So, for any chosen Q there is always a set of X_0 choices that will guarantee local robustness for σ_2. Now, if the segment is produced by σ_1 then $Q = Q_{max}$. Applying the same reasoning as before, and remembering that this is a finite-time horizon problem with bounded variables (*e.g.* $V_0 \leq V \leq V_f$) it follows that there is a choice set for Q_{max} that will guarantee local robustness for σ_1.

As a conclusion the Extended ED-TOC is always hovering and, for any given robust zone, it is always possible to choose some X_0 and some Q_{max} for making it also robust.

As example, a BP process generates a Gaseous Product (GP) modeled by Equation (10) (Dochain and Vanrolleghem, 2001; Titica *et al.*, 2003). It may replace y, in Fig. 7B, as $y = y_{GP}$, in order to multiply it by the volume level before feeding the ESS. Note that the ESS does not need to know the value of any model parameter *i.e.* the ED-TOC is completely robust to model uncertainties.

Equation (10) $$y_{GP} = k_2 \mu X$$

For an aerobic WW process the DO is measurable and may be modeled by the mass balance in Equation (11) (Dochain and Vanrolleghem, 2001). For this case $y=O$ in Fig. 7B. After manipulating Equation (11) it is possible to calculate the Oxygen Mass Uptake Rate in Equation (12) in order to use it as input for the ESS, with the additional advantage that, for the toxicant WW case, biomass growth is extremely slow compared to the biotechnological BP case.

Equation (11) $$\frac{dO}{dt} = -(k_3\mu + b)X + k_L a(O_{sat} - O) - (O - O_i)\frac{Q}{V}$$

Equation (12) $$OMUR = (k_3\mu + b)B = \left(k_L a(O_{sat} - O)) - (O - O_i)\frac{Q}{V} - \frac{dO}{dt}\right)V$$

Note that it is not necessary to know k_3, b nor B. In this case it is necessary to use only 3 parameters of the model (k_La, O_i and O_{sat}) to compute the right hand side of Equation (12), and all of them are easy to obtain with precision. The only concern may be the computation of the derivative. However, as the dissolved oxygen is a low frequency signal, by using finite differences numerical methods, including noise rejection filters, it is possible to obtain a good practical approximation.

Practical ED-TOC

In the prior subsection it was explained how minor errors in estimating the events, caused by a perturbation (*e.g.* the biomass growth) in the measured signal, would not significantly degrade the ED-TOC performance. However there are other possible sources of perturbation that might also cause estimation errors. This subsection is devoted to proposing practical solutions to such inconveniences:

- *pH, Temperature, DO limitation, and similar perturbations*. Over the duration of one reaction, μ is affected by changes in Temperature, pH, DO (for aerobic reactions) and many other factors. Such variations may be modeled as $\gamma = \mu_t(t)\, \mu_{pH}(t)\, \mu_T(t)\, \mu_{DO}(t)$, a format similar to the one studied for the extended ED-TOC in the previous subsection. ED-TOC robustness is kept if such perturbation effects are small *i.e.* if the errors are bounded. If that is not the case then a different independent control loop must be applied to reject the perturbation, or a redesign could be needed. For example, in the toxicant WW case, DO dropping near zero becomes a limiting factor for the reaction and μ_t is masked by μ_{DO}

effects, thus rendering γ useless for the ESS. In that case aeration must be increased (maybe by an independent control loop augmenting k_La) or biomass concentration reduced (a redesign).

- *Sensor inaccuracy*. So far it has been assumed that measured signals were exact and noise free. The fact is that in practical applications this is far from true. However inaccuracy poses no problem because, as it was shown, the ESS works with relations rather than with absolute values.

- *Noise*. In case noise is expected filtering is required. But even then some noise effect remains anyway. If its effect is not negligible a possible course of action is tuning P. Note that by making P closer to one, the ED-TOC becomes more sensitive to small signal changes, *i.e.* sensitive also to noise affecting such a signal. Then it is possible to reduce noise sensitivity by reducing P, *i.e.* a compromise for the width of the near-optimal zone must be met.

- *Time Delays*. The simplified model in Equations (1-3) assumes that when the input bounces between its bang-bang limits, *i.e.* Q is switched ON/OFF or OFF/ON, the S derivative (and the tendency of related variables) changes sign immediately *i.e.* the fast dynamics for tank equalization and the sensor delays are not considered. The ESS relies on such an assumption to work properly. Table III presents two ways to solve the delay problem as an integral part of the ED-TOC implementation: *Option 1* idea is that once the k^{th} state change is produced, at time t_k, the ESS will wait some T_s stabilizing time before taking any other new decision, *i.e.* before generating a new event, thus giving enough time for the fast non modeled dynamics to disappear after each state transition; *Option 2* requires that a condition to trigger an event holds at least for some T_s lapse before accepting it as valid. Both options establish a minimum switching time for the bang-bang cycle, *e.g.* T_s, thus limiting the minimum width selectable for the near-optimal zone. But such a compromise may not be really a concern as a minimum switching time is also desirable in order to protect actuators from chattering effects.

- *Non inhibitory substrates*. In such a case the SBR is non optimizable (Assumption 2). However, the ED-TOC will still behave in the best possible way by filling the SBR in a single bang (FTC like).

- *Shock loads*. High input concentrations are no problem for the ED-TOC as long as the generated dynamics could be followed by the sensors. Such a case is especially important for the toxicant WW treatment, where the unknown and unmeasurable toxicant concentration is expected to be in a certain range but, in some cases and without warning, it might increase to shock peak values.

APPLICATIONS

In order to avoid actuator wearing, the ON/OFF cycling was chosen to be less than 3 cycles per hour. This leaded to tune P=0.86 in the WW case and P=0.99 in the BP one.

Toxic Wastewater (WW) Treatment Case

In order to study performance differences between ED-TOC and FTC, different inflow concentrations were comparatively treated. The standard influent toxic concentration was S_{std} = 0.35 g4CP/L. Using the FTC, twice such a value would greatly inhibit the biomass thus preventing the treatment to be completed, and higher shock loads might even stress and/or disable the biomass permanently (Buitrón *et al.*, 2003). As a consequence it was necessary (for the FTC case only) to pre-dilute the influent in order to obtain the standard concentration for the inflow, thus a series of standard reactions was required to treat the shock loads. Results in Table IV show that the ED-TOC, able to treat the influent without neither diluting nor measuring it, increases significantly the daily applicable load: 85%, compared to the FTC in standard conditions, and in excess of 63% for the perturbing increasing shock loads. Removal efficiencies for 4CP were always superior to 99% and COD varied between 96 and 98%. As the time spent for treatment was less than for FTC, more than 25% energy savings in stirring and aeration were always observed for the ED-TOC.

Fig. 8 shows one experimental kinetic for a shock load case of S_i= 2S_{std}, using Equation (12) for implementing the ED-TOC. Toxic concentration S was registered offline (see 4CP in Fig. 8, square marks) from manually taken samples, and was not used for control purposes. Fig. 8 shows that S was kept oscillating in an acceptably low concentration range, by properly turning ON or OFF the inlet flow (Fig. 8, continuous thick gray line). Some perturbation came from the online sensor used to measure DO (Fig. 8, dotted line). It introduced second order delay effects, and some noise, reflected when calculating the OMUR for using it in the ED-TOC. But thanks to the ESS robustness (using option 1 in Table III with T_s=5min), the ED-TOC did cope smoothly with that perturbation.

Biomass Production (BP) Case

In this case the ED-TOC objective is to obtain the maximum amount of biomass, equal to that produced by using the nominal TOC, but spending less than 2% extra time. Each scenario in Table V provides a different challenge to the ED-TOC. The first one was defined as the nominal case, with no perturbations. In the second one the gaseous production sensor is badly calibrated. Its readings are 20% higher than the nominal value. Fig. 9 shows the simulation results for the last one, where a 100% shift in S^* happens during part of the reaction. Even then the optimality index ($t_{f.opt}/t_f$) was greater than 99% (Table V) *i.e.* the necessary time to complete the reaction objective was just slightly greater than the one needed by the exact TOC in ideal conditions. Results are as good as the ones for the Adaptive Extremum Seeking controller (Titica *et al.,* 2003). However ED-TOC robustness was better: it does not need the substrate to be measured neither in the influent nor in the tank; and it behaved practically optimally although no information about any process parameter was given to it, and while subjected to sensor inaccuracy and to process changes. This suggests the possibility of using the ED-TOC for optimizing any generic BP process conforming to Assumption 1 and Assumption 2.

CONCLUSIONS

An *Event-Driven Time-Optimal Control* (ED-TOC) strategy was proposed for minimizing the filling and reaction time in discontinuous bioreactors performing a single biomass growth process. Time minimization allows energy savings and also performing more batches per time unit. The main advantage of this strategy is that substrate and biomass concentrations measurements are not needed. It uses a variable, practically measurable, indirectly associated to the reaction rate *e.g.* a gaseous product production rate, or, for aerobic processes, the DO concentration. If some natural conditions for the problem are assumed, few parameters from the process model, if any, are required.

It was shown how to tune the ED-TOC and how to design the process, in order to robustly make it time-optimal, for any given bounded perturbation effect.

Another advantage of the ED-TOC is that a simple ON/OFF pump will do, because the filling proceeds as if mini *fill-react* batches were successively performed, i.e. inflow is pumped in until the event *"there is inhibition"* is detected, and then stops. When the biomass consumes the newly added substrate to the point where *"there is no inhibition*", a new pumping mini cycle begins. Such a bang-bang cycling continues until the reactor gets full.

An experimental application, treating toxicant wastewater modeled with 4-chlorophenol, was performed in a lab-scale reactor. Only DO and Volume level were used by the ED-TOC. Results show energy savings in excess of 25% and a daily applied load increase of 85%, in standard conditions, compared to the Fixed Time Control batch strategy, and more than 63% for perturbing shock loads, up to 20 times the standard conditions.

Another case, a biomass production process, was studied in simulation. The only variables measured were a gaseous product production rate and the Volume level. Not a single parameter of the process was needed by the ED-TOC to robustly obtain a practically minimum processing time.

ACKNOWLEDGEMENTS

Thanks to CONACyT (Project 34934A) and DGAPA for its financial support. This paper includes results of the EOLI project.

Manuel Betancur thanks UPB, CESAME, and Mariana Titica for helping setting up the scenarios for the BP simulation, and for her insights about the ED-TOC vs. Adaptive Extremum Seeking methods.

The scientific responsibility rests with the authors.

NOMENCLATURE

b	(h^{-1})	Specific endogenous respiration rate
B	*(gVSS)*	Total Biomass. Restricted by $B>0$
E_k	*(h)*	Error estimation of the event causing the k^{th} state transition

e_m		m type event, m=0, …, 5
k_n		yield coefficients, n=1, …
k_La	(h^{-1})	Oxygen mass transfer coefficient
O	*(mg/L)*	Dissolved Oxygen concentration inside the reactor. Restricted by $0 \leq O \leq O_{sat}$
Q	*(L)*	Inlet rate, the manipulated control variable. Restricted by $0 \leq Q \leq Q_{max}$
S	*(g/L)*	Substrate concentration inside the reactor. Restricted by $S \geq 0$
S^*	*(g/L)*	Concentration of the substrate at which μ is maximum
T_E	*(h)*	Escaping Time (from near-optimal into outside the robust zone)
t_k	*(h)*	time at which the k^{th} state change is produced
T_k	*(h)*	time duration of the k^{th} segment of the space-state trajectory
T_R	*(h)*	Returning Time (from the robust frontier into the near-optimal zone)
T_s	*(h)*	time allowance for signals to stabilize
V	*(L)*	Volume level of the liquid medium in the tank. Restricted by $0 \leq V_0 \leq V \leq V_f$
X	*(gVSS/L)*	Biomass concentration. Restricted by $X > 0$

Greek Symbols

μ, μ_t	(h^{-1})	Specific biomass growth rate. *S* dependant and *time* dependant, respectively
μ^*	(h^{-1})	Maximum specific growth rate
σ_n		n type logical state for the ED-TOC during fill and react phases: n=0, …, 4
φ		Time-varying upper bound for γ
γ		Measurable or computable function of μ

Subscripts and Underlining

0, i, f, opt, sat and *std* are used for *t*=***0*** *(initial),* ***i****nflow,* ***f****inal,* ***opt****imal,* ***sat****uration* and ***st****an****d****ard*.

Underlined names identify uncertain values. These differ from nominal ones by an unknown bounded quantity, possibly because they have been identified, estimated, measured and/or perturbed.

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TABLES AND FIGURES

EVENT-DRIVEN TIME-OPTIMAL CONTROL FOR A CLASS OF DISCONTINUOUS BIOREACTORS

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Table I. Finite States for the ED-TOC (for all implementation versions)

State	Tag	e_m/σ_n (if e_m go to σ_n)	Description	Control Action
σ_0	test	e_0/σ_1, e_3/σ_3, e_5/σ_2	find out what are the initial conditions	$Q=Q_{max}$
σ_1	fill	e_1/σ_2, e_3/σ_3	fill until inhibition appears	$Q=Q_{max}$
σ_2	wait	e_2/σ_1	wait until inhibition disappears	$Q=0$
σ_3	full	e_4/σ_4	wait until the reaction ends	$Q=0$
σ_4	end		may go to next phase *i.e.* settling	$Q=0$

Table II. Relevant Events for the ED-TOC implementation

Event	Meaning	Description	Event estimator function
e_0	$S < S^*$	there is no inhibition	$Q>0$ and $d\gamma/dt > 0$
e_1	$S \geq S_{high}$	there is inhibition and reaction rate is below near-optimal limit	$Q>0$ and $\gamma \leq P\gamma^*$ and $d\gamma/dt \leq 0$
e_2	$S \leq S_{low}$	there is no inhibition but reaction rate is below near-optimal limit	$Q=0$ and $\gamma \leq P\gamma^*$ and $d\gamma/dt \leq 0$
e_3	$V \geq V_f$	the tank is full	$V \geq V_f$
e_4	$S \leq S_f$	terminal substrate concentration reached *i.e.* it is in the finishing zone	$Q=0$ and $\gamma < R\gamma^*$
e_5	$S > S^*$	there is inhibition	$Q>0$ and $d\gamma/dt<0$

Table III. Event estimator functions robust against non modeled fast dynamics

Event	Meaning	Event estimator function (option 1)	Event estimator function (option 2)
e_0	$S < S^*$	$Q>0$ and $d\gamma/dt>0$ and $t \geq t_{k-1}+T_s$	($Q>0$ and $d\gamma/dt>0$) for at least T_s seconds
e_1	$S \geq S_{high}$	$Q>0$ and $\gamma \leq P\gamma^*$ and $t \geq t_{k-1}+T_s$	($Q>0$ and $\gamma \leq P\gamma^*$) for at least T_s seconds
e_2	$S \leq S_{low}$	$Q=0$ and $\gamma \leq P\gamma^*$ and $t \geq t_{k-1}+T_s$	($Q=0$ and $\gamma \leq P\gamma^*$) for at least T_s seconds
e_3	$V \geq V_f$	$V \geq V_f$	$V \geq V_f$
e_4	$S \leq S_f$	$Q=0$ and $\gamma < R\gamma^*$ and $t \geq t_{k-1}+T_s$	($Q=0$ and $\gamma < R\gamma^*$) for at least T_s seconds
e_5	$S > S^*$	$Q>0$ and $d\gamma/dt<0$ and $t \geq t_{k-1}+T_s$	($Q>0$ and $d\gamma/dt<0$) for at least T_s seconds

Table IV. Comparison of applicable load for the ED-TOC versus FTC

S_i (S_{std}=0.35g4CP/L)	Daily Load (kg COD/m^3/d)			Applied Load increment (%)
	FTC Undiluted (S_i as it is)	FTC Pre-diluted to standard	ED-TOC Unknown and undiluted	ED-TOC vs. pre-diluted FTC
S_{std}	2.52	2.52	4.65	85
2 S_{std}	Not Possible+	2.52	4.58	81
8 S_{std}	Not Possible*	2.52	4.11	63
14 S_{std}	Not Possible*	2.52	4.80	90
20 S_{std}	Not Possible*	2.52	4.77	89

+The standard FTC time is not enough for achieving total mineralization (Buitrón *et al.*, 2003).

*The SBR gets disabled if $S_i > 1.05$ g4CP/L in FTC mode (Buitrón *et al.*, 2003).

Table V. ED-TOC Optimality results for different scenarios in the Biomass Production case

Scenario	Description of the test conditions for ED-TOC simulation	Optimality index $t_{f.opt}/t_f$ (%)
1	Nominal case with Haldane law defined as in Titica *et al.* (2003) $\mu_o=0.53\ K_I=0.22\ K_S=1.2\ (S^*=0.5138)$	99.8
2	Measurement error of the gaseous product production rate of +20% in t=(20,30)	99.8
3	Perturbation of μ *i.e.* S^* not constant. It increases 100% during $t=(20,50)$	99.1

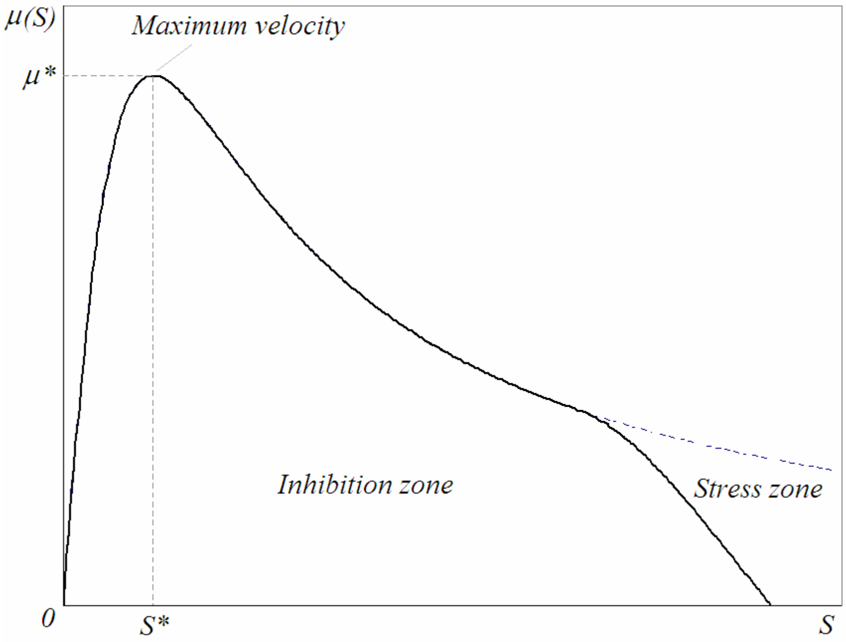

Fig. 1. Inhibitory Biomass Specific Growth Rate

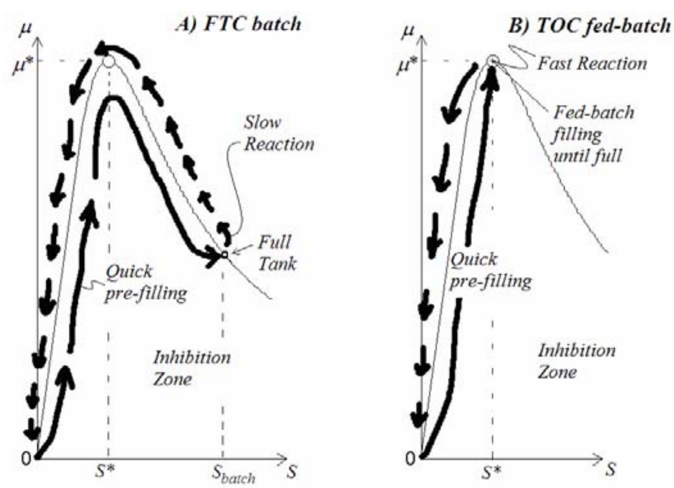

Fig. 2. $\mu(S)$ evolution as S varies during the filling and reacting:

A) Fixed Time Control (FTC) batch; B) Time Optimal Control (TOC) fed-batch

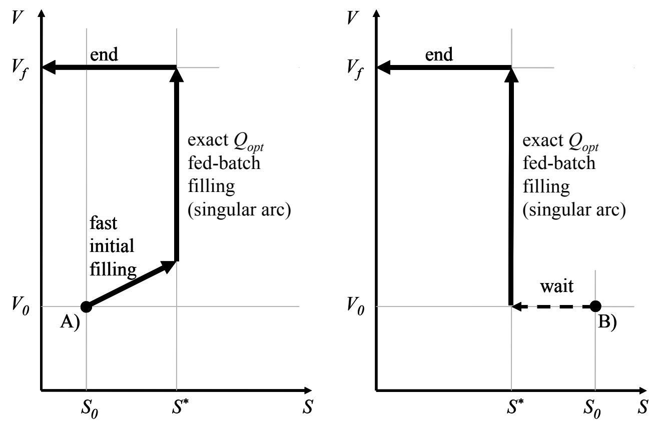

Fig. 3. *SV* projection of the TOC trajectory:

A) $S_0 < S^*$; B) $S_0 > S^*$

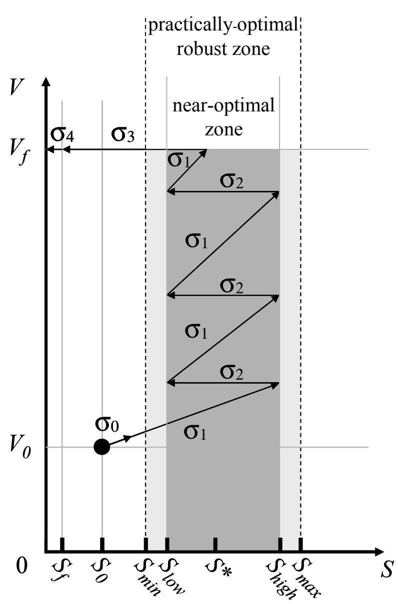

Fig. 4. *SV* projection of the ED-TOC Trajectory (for $0<S_0<S^*$)

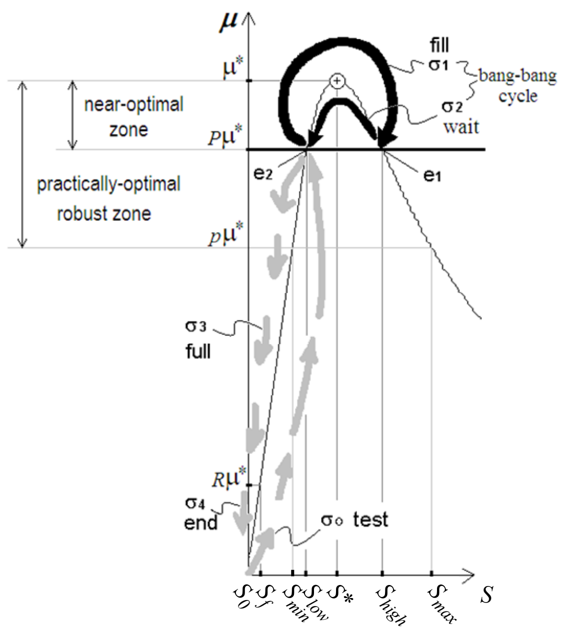

Fig. 5. S evolution in ED-TOC mode (for S_0=0)

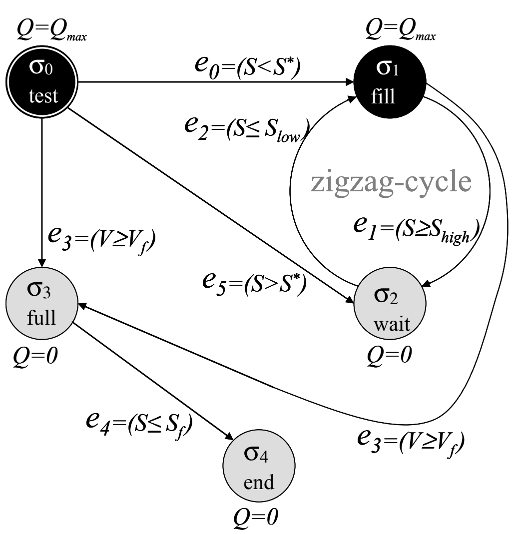

Fig. 6. Finite states transitions diagram of the ED-TOC

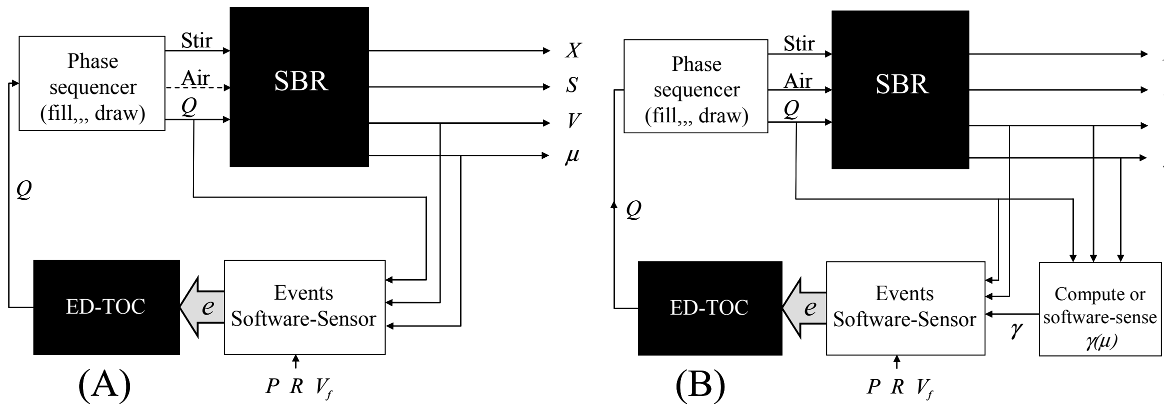

Fig. 7. ED-TOC layout:

A) using the non measurable $\mu_t(t)$; B) using a computable $\gamma(t)=f(\mu_t(t))$

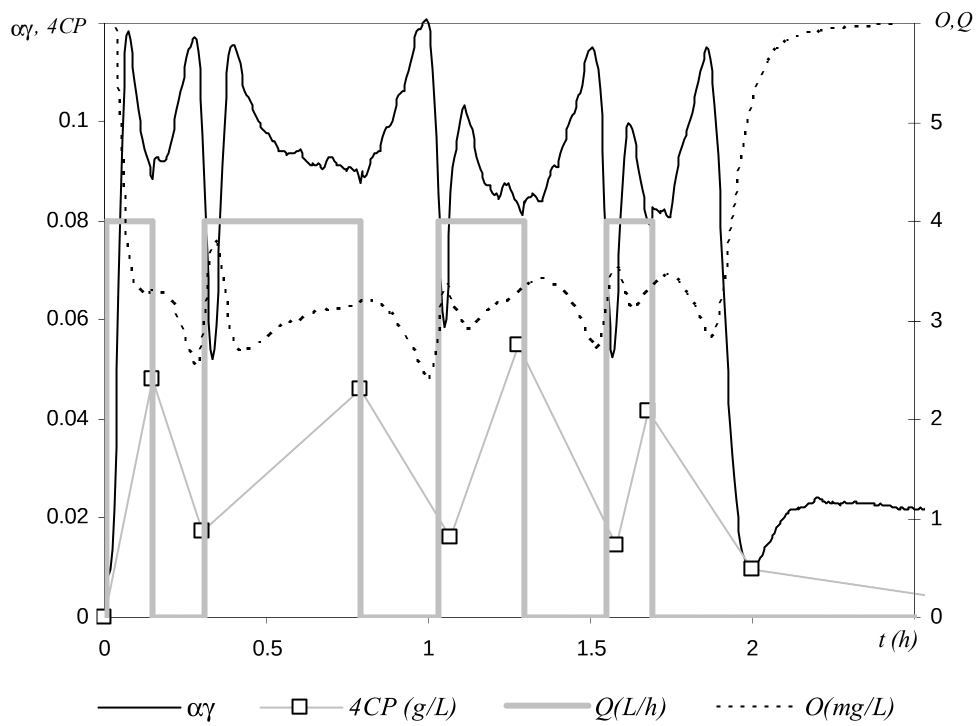

Fig. 8. Experimental kinetics using the ED-TOC to control a lab-SBR.

A 4CP shock load, twice the standard value (S_i=2S_{std}), is treated using B_0=14 gVSS.

Note that γ [*i.e.* the OMUR, computed online using the DO (dotted line) measurement] was scaled by a constant (α) just to fit the graph (and to remove units). Its shape (thin continuous line), however, remains the same. Offline substrate samples (square marks) were taken every time the ED-TOC switched the pump. Note that always, soon after *Q* switches (thick gray line), γ begins to increase. That is just what the ED-TOC looks for, to try to maximize γ. The cue for switching the pump, again, is to wait for γ to reach a peak (γ^*) and then to decrease to the predefined $P\gamma^*$ threshold. At that point the ED-TOC knows that γ tendency is not good (biomass activity is decreasing) and so it switches *Q* to change such a tendency.

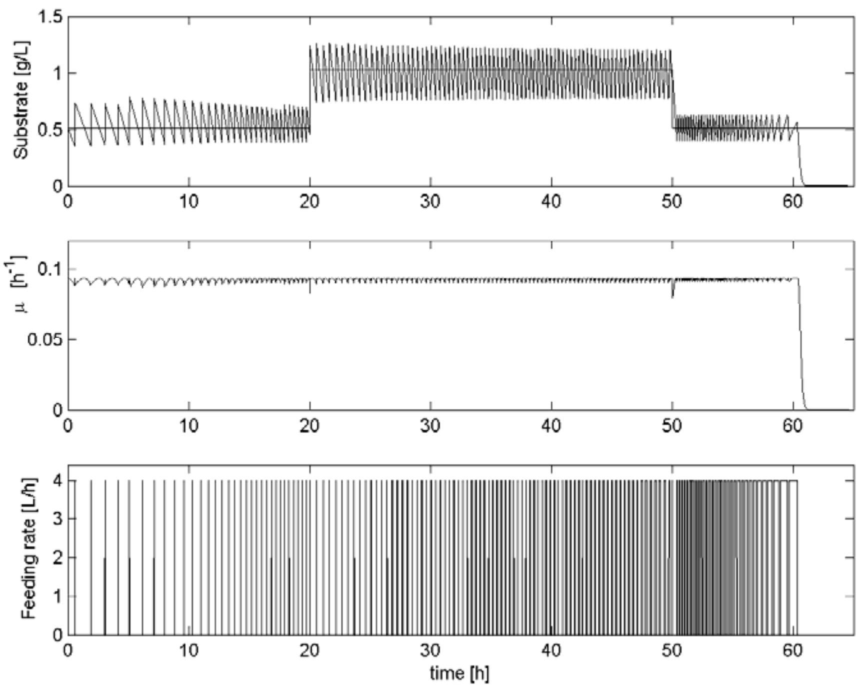

Fig. 9. ED-TOC simulation results for the Biomass Production case using settings from scenario 3 in Table I