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Application of the event-driven time optimal control strategy for the degradation of inhibitory wastewater in a discontinuous bioreactor

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Abstract: This work presents the results of the application of a new control strategy to optimize the degradation rate of toxic compounds. The event-driven time optimal control strategy (ED-TOC) was applied to biodegrade in a discontinuous reactor (SBR) a synthetic wastewater constituted with 4-chlorophenol (4CP) as model of the inhibitory compound. The ED-TOC strategy was developed in a manner to estimate a variable (named gamma) related to the substrate degradation rate in such a way that maximizing the former, the later is maximized too, but without measuring it. Gamma can be estimated in real time by using the dissolved oxygen concentration and the volume of the reactor. In the ED-TOC strategy, the influent flow rate is controlled in such a manner that the substrate degradation rate stays around its maximal value. To estimate gamma, only the mass transfer coefficient and the dissolved oxygen concentration at saturation are needed. It was found that a practical implementation of the ED-TOC strategy was possible. The degradation and mineralization of the 4CP were efficiently achieved. The average removal efficiencies were 99%, as chemical oxygen demand and 100% as 4CP. Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h. The ED-TOC strategy was able to manage increments of toxic concentrations in the influent up to 11200 mg 4CP/L. It was shown that not only higher concentrations of toxic could be treated with the ED-TOC strategy, but also a reduction in degradation time was obtained. For a given initial concentration of 4CP, the degradation rate was higher (almost doubled) with the ED-TOC strategy than the reaction rate obtained with the usual operation mode utilized in the SBR.

Introduction

The activated sludge process has been traditionally applied to treat industrial wastewater, but the nature of such discharges often causes operational problems in continuous flow systems. This is the case of the wastewaters containing toxic compounds generated by several chemical and petrochemical facilities. In such streams the mass of toxic contaminants varies with either time or space. Recently, innovative strategies like the discontinuous processes (controlled unsteady state processes) have been explored in order to increase the biotreatment efficiencies of wastewater (Buitrón *et al.* 2001). The term Sequencing Batch Reactor (SBR) is used as a synonym of the wastewater treatment technology where the volume of the reactor tank is variable in time (Wilderer *et al.* 2001). It can work with suspended or attached biomass. In general, the SBR process presented three major characteristics: periodic repetition of a sequence of well defined phases; planned duration of each process phase in accordance with the treatment result to be met and progress of the various biological and physical reactions as a function of time. Another characteristic of the SBR systems, because of their flexibility in control strategy, is that they are effective for fully automated computer controls.

Usually a SBR-type bioreactor operates under five well-defined phases: fill, react, settle, draw, and idle. The way in which the duration of each one of these phases is determined can be denominated operation mode and has a fundamental impact in the SBR characteristics. In the standard operation mode, the duration of these phases is typically determined by an expert operator based on his experience and exhaustive testing in the laboratory with a pilot plant. In particular, the reaction phase is sufficiently long to allow the toxic substances being degraded. The settle and draw phases are fixed in duration by the characteristics and constraints of the activated sludge and the reactor itself. Thus, this operational strategy could be considered as Fixed Timing Control strategy (FTC). Despite the inherent advantages of the discontinuous processes in relation to de biodegradation of toxic substances, the SBR operated under the FTC present several constraints when they are applied to the toxic wastewater degradation: inhibition of the microorganisms, problems with shock loads of toxic compounds, deacclimation and problems of starvation of the microorganisms and low efficiencies regarding the removal of toxic compounds (Buitrón and Moreno 2002; Buitrón et al, 2003).

To overcome the problems discussed above several operation modes have been presented using either dissolved oxygen (DO) concentration or the carbon dioxide evolution rate (CER) (Sheppard and Cooper, 1990; Buitrón *et al.* 1993; Nguyen *et al*., 2000). Moreno and Buitrón (1998) presented a methodology and mathematical simulations for the time optimal control of an activated sludge sequencing batch reactor (SBR) for toxic wastewater degradation. The optimal strategy for the input flow was obtained using techniques of optimal control theory, in which the reaction time is as small as possible. The degradation time was controlled through the substrate concentration estimated from the liquid oxygen concentration using an observer (Extended Kalman Filter). Vargas *et al.* (2000) presented the calibration of the observer and the experimental validation the Observer-Based Time Optimal Control strategy (OB-TOC). The drawback of this strategy is that it needs to know exactly the inflow substrate concentration and the constants of the Haldane model. This could make the OB-TOC difficult to apply in practice. Betancur *et al.,* (2004) described the mathematical development of a new Event-Driven Time Optimal Control strategy (ED-TOC) that measures the dissolved oxygen to robustly control the reaction rate of a discontinuous process treating inhibitory compounds.

This work presents the results of the application of the ED-TOC strategy to biodegrade, in a discontinuous reactor, a synthetic wastewater constituted with 4-chlorophenol as model of the inhibitory compound.

Methodology

Event-Driven Time Optimal Control Strategy

The ED-TOC strategy finds a variable (named γ) related to the reaction rate. Such variable can be estimated in real time by using the dissolved oxygen concentration and the volume of the reactor, as it was described in detail by Betancur *et al.* (2004). It is known that the behavior of the biomass growth rate (μ) as a function of the toxic substrate concentration (S) can be described by the Haldane law. In this model, μ reaches a maximal value, μ^*, when the substrate concentration is S^*. Toxic concentrations above or below μ^* will generate a diminution in the growth rate and, consequently, also in the reaction rate. Thus, if it is guaranty that S is near to S^*, it is also possible to maintain the degradation rate near to a maximal value. The problem consist, therefore, in to bring and to maintain μ at its maximal value during all the reaction period of the reactor. An additional problem is that μ is as much or more difficult to measure on-line in practice than the substrate concentration. It is interesting to point out that in the ED-TOC strategy it was developed a manner to estimate γ related to μ in such a way that maximizing the former, the later is maximized too, but without measuring it. In this case γ is proportional to μ by an unknown constant, which is not necessary to know for control purposes. Betancur *et al.* (2004) explained in detail how equation 5 was obtained from the model of a discontinuous reactor (equations 1 to 4):

$$\frac{dX}{dt} = \mu X - K_d X - X\frac{Q_{en}}{V} \qquad (1)$$

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}}\mu X + \left(S_{en} - S\right)\frac{Q_{en}}{V} \qquad (2)$$

$$\frac{dO}{dt} = -\frac{1}{Y_{X/O}}\mu X - bX + K_l a\left(O_s - O\right) + \left(O_{en} - O\right)\frac{Q_{en}}{V} \qquad (3)$$

$$\frac{dV}{dt} = Q \qquad (4)$$

$$\gamma = \frac{XV}{Y_{X/O}}\mu + bXV = K_l a\left(O_s - O\right)V - OQ_{en} + V\frac{dO}{dt} \qquad (5)$$

where,

***X*:** Biomass concentration inside the reactor; ***S*:** Substrate concentration inside the reactor; ***V*:** Water volume level in the reactor; ***O*:** Dissolved oxygen concentration, **$Y_{X/S}$:** Biomass/substrate yield coefficient; **$Y_{X/O}$:** Biomass/oxygen yield coefficient; **$K_l a$:** Oxygen mass transfer coefficient; ***b*:** Specific endogenous respiration rate; **K_d:** Decay biomass rate; **μ:** Specific growth rate, **S_{en}:** Influent substrate concentration; **O_{en}:** Influent dissolved oxygen concentration; **Q_{en}:** Influent flow rate; **O_s:** Dissolved oxygen concentration at saturation; γ: variable proportional to **μ**.

Using the ED-TOC strategy, the influent flow rate is controlled in such a manner that the reaction rate stays inside the fast zone (gray zone in Figure 1). Such zone is above a P% of the maximum rate. The reaction rate is controlled maintaining the substrate concentration oscillating in a gap during the SBR filling. Every time the substrate concentration tries to leave this gap, an event is issued and the ED-TOC then switches the influent flow on/off, to prevent it. This will work regardless of the substrate influent concentration value and despite changes in most of the SBR parameters. All the variables in the right side of equation 5 are measurable or straightforwardly computable. Only the mass transfer coefficient, $K_l a$, and the dissolved oxygen concentration at saturation, O_s, are needed to estimate γ and they do not even need to be known precisely. This solution is therefore a good candidate for uses in real industrial environments.

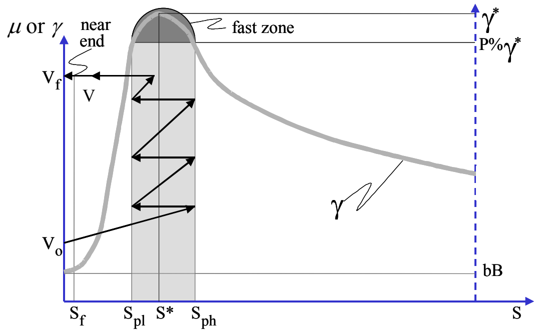

Figure 1 Plan trajectory for the ED-TOC strategy. Vo indicates the initial volume in the tank. The flow is feed to the reactor in such a manner to keep the reaction rate around the optimal value (gray zone). Once the final volume is reached, V_f, the reactor acts as a batch process and the reaction rate decreases.

Pilot reactor

An aerobic automated Sequencing Batch Reactor (SBR) system with a capacity of 7L and an exchange volume of 57% was used (Figure 2). The airflow rate was 1.5 liters per minute and the temperature was maintained at 20 ºC inside the reactor. The reactor was inoculated with microorganisms coming from a municipal activated sludge treatment plant (2000 mgVSS/L). A synthetic wastewater containing (4CP) was used as a sole source of carbon and energy. For standard conditions reactor was operated using an influent concentration of 350 mg 4CP/L. The strategy was tested using different initial concentrations of 4CP between 175 and 11200 mg/L, and also different airflow rates (0.75, 1.5 and 2.25 lpm). Nutrients such as nitrogen, phosphorus, and oligoelements were added following the techniques recommended by ANFOR (1985). The SBR was operated under the following strategy (except for acclimation period that is described above): preaeration time (15 min), filling and reaction time (variable depending on the influent concentration), settling time (30 min) and draw time (6 min).

Analytical methods

The substrate concentration was measured taking samples and processing them offline using the colorimetric technique of the 4-aminoantipyrine method (Standard Methods, 1992). Total and volatile suspended solids (TSS and VSS) analyses were determined according to the Standard Methods (1992). Dissolved organic carbon (DOC) was determined with a Shimadzu TOC-5050 and Chemical Oxygen Demand (COD) according to Standard Methods (1992). Theses analyses were performed to evaluate the 4CP mineralization. The metabolite (5-chloro-2hydroxy-muconic acid semialdehyde) (Commandeur and Parson, 1990), formed by an alternate degradation route of 4-CP by the microorganisms, and that can be inhibitory for the microorganisms, was also determined by spectrophotometry at 380 nm using a HACH spectrophotometer. Specific oxygen uptake rate (SOUR) experiments were conducted placing 10 mL of the mixed liquor of the SBR harvested just after a degradation cycle in a mini-reactor of 160 mL. An oxygen-saturated solution with nutrients and substrate (acetate or 4CP) was added and dissolved oxygen measured was recorded. Endogenous respiration was measured adding only nutrients. SOUR was computed from the slope of the reprogram divided by the VSS concentration.

Figure 2 Pilot reactor utilized for the toxic compounds degradation

Results and Discussion

Biomass Acclimation

The biomass was acclimated using a variable cycle strategy, i.e., the reaction phase duration was variable and stopped when the removal of 4CP was equal or greater than 95%. Acclimation was done using an initial 4CP concentration of 175 mg/L in the influent. When degradation time was constant, initial concentration was doubled and, then the reactor was maintained operating at 350 mg/L under the ED-TOC strategy. Figure 3 presents the evolution of the initial and final COD, as well as the TSS in the effluent. The average removal efficiency was 99%, as COD (483 and 5 mgDCO/L at influent and effluent, respectively) and 100% (as 4CP). Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h. These data indicate a good performance of the reactor operated with the ED-TOC strategy.

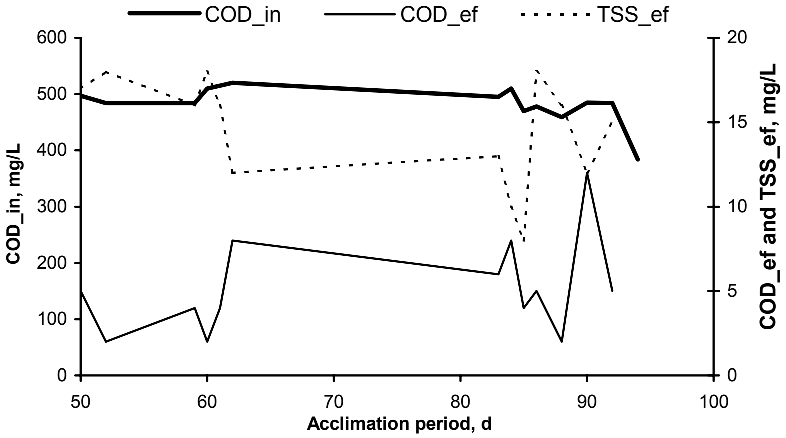

Figure 3 Evolution of the COD at the influent and effluent and TSS at the effluent for the process operated under the ED-TOC strategy.

Standard Conditions Kinetics

Figure 4 presents the behavior of the substrate concentration, measured as 4CP, COD, and DOC during a cycle operated under the ED-TOC strategy. It is possible to distinguish how the control operates following the substrate and the DO evolution curve. Once the influent begins to be fed to the reactor, the reaction starts. The DO decreases (first 0.2 h, figure 4) as the metabolic activity of the biomass increases to degrade the 4CP. Simultaneously, the estimator calculates γ and follow its value. When a maximal point is detected (before a minimum in the DO concentration), the feeding pump is turned off. In this point, the concentration of substrate is low than expected (it passed from 48 to 22 mg4CP/L, at 0.4 h in figure 4). Thus, the feeding pump is switched on, and a new charge of substrate is fed to the reactor. This procedure is repeated until the maximal volume has reached and then, the degradation proceeds in a batch manner. It is possible to observe in Figure 4 how the internal concentration of the reactor is maintained around 30 mg/L, which corresponds to a concentration close to S* and thus, around μ*. The metabolite production increases as the reaction took places, but after the cycle has finished, the metabolite concentration decreases, indicating a good operation of the system.

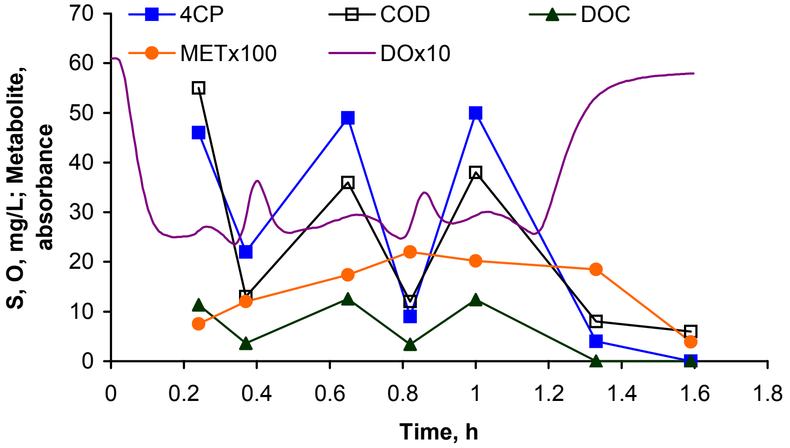

Figure 4 Evolution of the substrate concentration, measured as 4CP, COD, and DOC during a cycle operated under the ED-TOC strategy.

Performance of the ED-TOC strategy under different initial concentrations

In order to test the performance of the ED-TOC strategy in front of sudden incomes of concentration peaks to the plant, several initial concentrations of 4CP were tested. The performance of the reactor is compared to the response obtained by the reactor operated under the fixed timing strategy (FTC), a standard operation mode of the SBR. Table 2 summarized the results obtained. The reactor operated under the FTC strategy was able to manage concentration peaks up to 760 mg/L in the influent with an increment in the degradation time of 50%. In this case, it was necessary a week to recover the previous performance. Higher concentrations generated a severe problem of inhibition to the biomass. On the contrary, the ED-TOC strategy was able to manage increments of concentration in the influent up to 11200 mg/L. In theory, this strategy could treat any initial concentration in the tank. It is easy to demonstrate that not only higher concentration of toxic could be treated with the ED-TOC operation mode, but also a reduction in degradation time is obtained. If an initial concentration of 4CP of around 550 mg/L is considered, from table 1 it is observed that a specific degradation rates of 21 and 46 mg 4CP/gVSS –h are obtained for the FTC and the ED-TOC strategies, respectively. The degradation rate almost doubled with the optimal strategy for a same initial concentration of toxic to be treated.

Table 1. Effect of different operational strategies on the reactor performance under peaks of concentration.

Control strategy	Peak of 4CP, mg/L (S_{in})	Removal efficiencies during the peak (% of 4CP)	Degradation rate during the peak (mg 4CP/gVSS -h)	Performance of the reactor after the peak
FTC	550	100	21.0	No problem
FTC	760	85	18.5	Degradation time increases 50%. One week to recover previous performances
FTC	900	63	21.4	Severe affectation to the reactor performance. One month to recover.
ED-TOC	440	100	48.4	No problem
ED-TOC	530	100	45.8	No problem
ED-TOC	634	100	60.4	No problem
ED-TOC	700	100	63.5	No problem
ED-TOC	1400	100	91.2	No problem
ED-TOC	2800	100	114.3	No problem
ED-TOC	5600	100	114.3	No problem
ED-TOC	11200	100	114.3	No problem

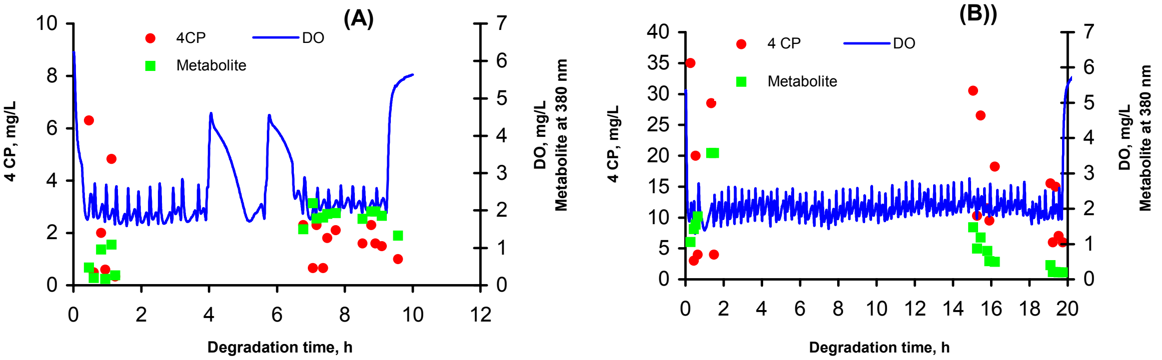

Figure 5 Degradation kinetics for an initial concentration of 2800 (A) and 5600 (B) mg 4CP/L using the ED-TOC strategy.

Dissolved Oxygen Variation

As the optimal strategy depends on the DO concentration to control the feed rate, it is important to study how much the variation in this parameter could affect the performance of the reactor. Two experiments were conducted varying the oxygen flow rate with respect to the standard value of 1.5 liters per minute. Figure 6 presents the evolution of the dissolved oxygen during the variation of ± 50 of the airflow in respect to standard conditions. For all the cases initial concentration of 4CP was 350 mg/L. When a –50% condition was applied, DO in the tank was always superior to 2 mg/L. Thus, it can be considered that no limitations for this element were present.

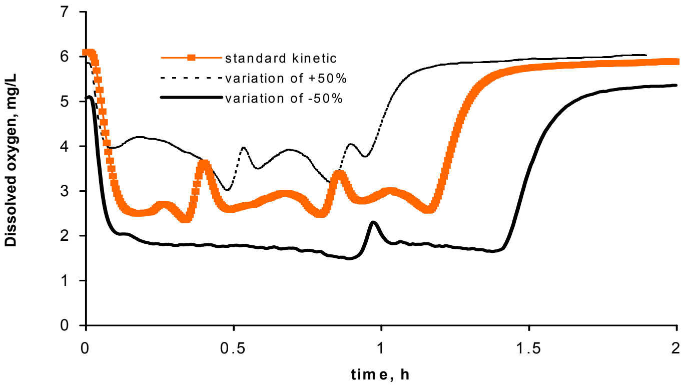

Figure 6 Evolution of the dissolved oxygen concentration as a function of time

Figure 7 shows the influence of the flow air variation on the substrate degradation (A) and on the metabolite production (B). In general, there was not a significant influence on the strategy operation when the air inflow rate was varied ± 50%. But, it is very interesting to note that in the case where the airflow was reduced by 50% there was an increase of the quantity of metabolite produced (Fig 7B). As a consequence, the degradation time for this same condition has a small increase (Fig 7A). Besides the influence on the metabolite production, this toxic by-product was no removed after the degradation cycle, which may cause problems due to the accumulation in the next cycles.

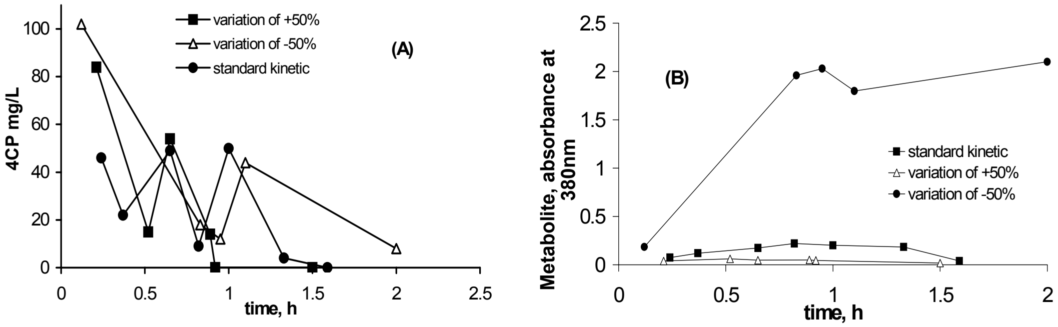

Figure 7 (A) Evolution during the degradation cycle of the 4CP concentration and the metabolite production (B) for different airflow rates

Conclusions

The application of a new control strategy to optimize the degradation rate of toxic compounds was presented. The event-driven time optimal control strategy (ED-TOC) was applied to biodegrade in a discontinuous reactor (SBR) a synthetic wastewater constituted with 4-chlorophenol (4CP) as model of the inhibitory compound. It was found that a practical implementation of the ED-TOC strategy was possible. A good performance of the reactor operated with the ED-TOC strategy was obtained since the degradation and mineralization of the 4CP was efficiently completed. The average removal efficiencies were 99%, as chemical oxygen demand and 100% as 4CP. Total suspended solids at the effluent were below 14 mg/L, sludge volumetric index around 38 ml/g, and settling velocity of the sludge of 6 m/h, which indicated the excellent settling characteristics of the sludge.

A better performance of the reactor operated with the ED-TOC strategy was observed when it was compared to the response obtained by the reactor operated under the fixed timing strategy. The ED-TOC strategy was able to manage increments of toxic concentrations in the influent up to 11200 mg 4CP/L without any problem. It was shown that not only higher concentrations of toxic could be treated with the ED-TOC strategy, but also a reduction in degradation time was obtained. For a given initial concentration of 4CP, the degradation rate was higher (almost doubled) with the ED-TOC strategy than the reaction rate obtained with the usual operation mode utilized in the SBR. In general, there was not a significant influence on the strategy operation when the air inflow rate was varied ± 50% in respect to the standard condition, but care must be taken when by-products are formed when aeration is not sufficient.

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