Practical automatic control of a sequencing batch reactor for toxic wastewater treatment
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ABSTRACT
This paper investigates the application of a practical and robust control strategy for the operation of a sequencing batch reactor (SBR) used for toxic wastewater treatment. The strategy sets the operational conditions of the SBR based on the on-line information collected during the previous batch. In particular, it sets the exchange volume of the reactor, as well as the batch reaction duration by optimizing the amount of mass of substrate in the influent treated per time unit. The optimization uses an experimentally calibrated mathematical model of the previous SBR cycle, found using the on-line dissolved oxygen concentration measurement data. The results show the applicability of the methodology to treat synthetic wastewater containing 4-chlorophenol as model toxic compound as sole source of carbon and energy. It correctly detects changes in the influent concentration and appropriately sets the operational parameters of the process.

Key words | automatic control, sequencing batch reactor, model-based control, toxic wastewater, 4-chlorophenol.

INTRODUCTION
Ever since the description of the operation of sequencing batch reactor (SBR) technology by Irvine & Davis (1971) its popularity and applications have substantially increased and received significant attention. Subsequent studies have fostered improvements to the technology, optimizing the performance of the system, e.g. two or more reactors can be used in a predetermined sequence of operations (Wilderer et al. 2001; Shaw et al. 2009).

SBRs are used and employed both for municipal and industrial wastewater treatment. Their relative compact size makes them suitable for small wastewater systems and for areas where there is a limited amount of space. This technology has a number of advantages and through the years many problems have been solved with better instrumentation, configurations, automation, variations in the mode of operation and new control strategies in order to achieve high efficiencies (Andreottola et al. 2001; Zangier et al. 2001). Cycles within the system can be easily modified for nutrient removal in the future, if it becomes necessary (Shaw et al. 2009).

An SBR is suitable for toxic wastewater treatment in the removal of specific organic compounds present in industrial wastewaters (Papadimitriou et al. 2009), in part thanks to the flexibility in the operational control strategy, which refers to the duration of its phases: fill, react, settle, draw and idle. The goals of the control strategy are to avoid death or inhibition of the microorganisms (inhibition affects the metabolic activity) caused by toxic compounds, to minimize or eliminate problems because of shock loads, and to increase the process efficiency even if there are disturbances.

The standard operation mode applied in SBRs is a fixed time control (FTC) strategy, with fixed durations for each phase. These are typically determined by an expert operator, based on experience and in-depth testing with a pilot plant in the laboratory; it uses no instrumentation to assess the terminal status, so there is no way to automatically finish the reaction phase (Moreno et al. 2006). Normally the fill is as rapid as possible while the duration of the react phase is long enough to allow the toxic substances to be completely degraded. The duration of the settle and draw phases is fixed by the activated sludge characteristics.

Some disadvantages of this strategy are: inhibition, problems with shock loads of toxic compounds, and deacclimation.
or starvation of the microorganisms. These problems cause a
direct impact on the process efficiency and make it imprac-
tical for the use under real operating conditions (Buitrón &
Moreno 2004); the strategy provides neither optimization nor
robustness for the process.

To overcome these problems and to obtain a robust
control strategy, several operation modes have been de-
veloped and proposed, depending on the application. Most use
on-line measurements of one or several process variables to
assess the state of the bioreactor. Some usual signals used
for this purpose are the oxidation-reduction potential, the
dissolved oxygen concentration (DO), or the oxygen uptake
rate (Shaw et al. 2009). In particular, assuming that the
biodegradation rate is proportional to the oxygen uptake
rate, the last two can be used to indicate when to stop the
reaction, such as in a variable time control (VTC) strategy
(Buitrón et al. 2005).

A further improvement is the event-driven time optimal
control (ED-TOC) strategy, where a controlled feed is imple-
mented such that the biodegradation rate is kept near its
maximum for most of the bioreaction. The SBR operation is
then robust enough to handle highly toxic influents, e.g.
concentration peaks or shock loads, since the resulting
pulse feeding keeps the concentration within the bioreactor
near an optimal non-inhibiting value (Moreno et al. 2006).

For an SBR degrading high concentration peaks of 4-
chlorophenol, it has been shown that the VTC strategy is not
efficient to control a bioreactor when there exist variations of
the concentrations of toxic organic compounds (Buitrón et al.
2005). The ED-TOC strategy handles these problems, but still
has the inconvenience from a practical point of view of
requiring a control loop, which is closed at all times by a
personal computer with data acquisition; in case of its failure
the process stops altogether, because decisions regarding
operation are being taken on-line. Furthermore, there might
be a significant delay in the calculation of the biodegradation
rate and the algorithm is susceptible to fail if its parameters
have not been properly calibrated.

The present work explores a different control paradigm.
Instead of using on-line information for taking decisions on
the current operating mode, these are determined a posteriori
using the collected data of the previous SBR cycle. A mathe-
matical model is calibrated and a criterion is optimized for
the next cycle. This way, even if some measurements are lost
during the previous SBR cycle (e.g. due to sensor failure),
the next cycle will not be compromised, in the sense that outliers
in the collected data can be discarded and the optimization
performed. If data are not trustworthy, the previous operating
conditions can be kept until repair of the failure.

MATERIALS AND METHODS

Pilot reactor and analytical methods

A fully automated aerobic SBR with 7 L of useful volume and
2 L of maximal exchange volume was used. The airflow rate
was 1.5 L/min (Aalborg GFC17 mass flow controller) and the
temperature was maintained constant at 20°C inside the reactor
by a recycling water pump. The input and output water flows
were controlled by means of peristaltic pumps, (Masterflex,
Cole-Parmer 7523-20 and 7553-30), which could be read
and controlled by the computer using solenoid valves. A DO sensor
and transmitter (Endress + Hauser COS41 and COM223) was
used to monitor this variable on-line. All signals were read and
written by a desktop computer with a data acquisition card
(USB6008, National Instruments) using LabView (Ver. 5.1)
software (National Instruments), which was also used to auto-
mate the reactor operation. Mathematical modelling and the
optimization procedure were carried out by calling an external
module programmed using Matlab (Ver. 7.5.0).

The reactor was inoculated with biomass from a munici-
pal activated sludge wastewater treatment plant (3000 ±
32.4 mgSSV/L). It was acclimated to degrade synthetic wast-
ewater containing 350 mg/L of 4-chlorophenol (4CP; Aldrich, purity ≥ 99.0%) as a sole source of carbon and
energy. This compound was used as a model of an inhibitory
compound due to its presence in wastewaters from different
industries. The acclimation was performed according to
Buitrón & Moreno (2004), starting with 100 mg/L of initial
4CP inside the reactor.

Nutrients (nitrogen and phosphorus) and oligo-elements
were added (AFNOR 1985). The standard mineral medium had
the following composition: 51 mg/L KH2PO4, 19.44 mg/L
K2HPO4, 150.9 mg/L Na2HPO4·7H2O, 58.26 mg/L NH4Cl,
22.5 mg/L MgSO4·7H2O, 36.4 mg/L CaCl2H2O, 0.25 mg/L
FeCl3·6H2O; and the trace compounds: MnCl2·4H2O,
H3BO4, ZnCl2 (NH4)6Mo7O24, EDTA, FeCl3·6H2O.

The 4CP concentration was measured (as total phenols)
taking samples and processing them off-line using a modi-
fication of the colorimetric technique of 4-aminoantipyrine
according to Standard Methods (2005). Total suspended
solids (TSS) and volatile suspended solids (VSS) analyses
were determined according also to Standard Methods
(2005).

Mathematical models

The model used for biodegradation of a toxic substrate
follows Haldane-type kinetics (Henze et al. 2008). If $X$
represents the biomass concentration and $S$ represents the substrate concentration, then for the fill and reaction phases the model is given by the following three differential equations:

$$\frac{dX}{dt} = \mu(S)X - k_dX - X \frac{Q_{in}}{V},$$

$$\frac{dS}{dt} = -\frac{1}{Y_{XS}}\mu(S)X + (S_m - S) \frac{Q_{in}}{V},$$

$$\frac{dS}{dt} = Q_{in}$$

(1)

where the specific biomass growth rate is given by a Haldane law:

$$\mu(S) = \frac{\mu_{max}S}{K_S + S + S^2/K_I} = \frac{\mu^* S S}{S^* S + \alpha(S^* - S)^2}$$

(2)

In the rightmost form, the two critical parameters, $\mu^*$ and $S^*$, which define the point where biomass growth is maximal, are explicit; the other parameter, $\alpha$, defines the form of the curve.

In the model (1)–(2) the biomass growth rate is proportional to the substrate biodegradation rate, which considers biomass inhibition, such that when the substrate concentration is above a certain level, the growth rate and hence the biodegradation rate decreases. However, it does not consider biomass sudden death from extreme intoxication at sufficiently high substrate concentrations.

On the other hand, the dissolved oxygen (DO) concentration dynamics has the following model:

$$\frac{dO}{dt} = \left(\frac{1}{Y_{XO}}\mu(S) - b\right) \left(\frac{O}{K_O + O}\right)X$$

$$+ (O_{sat} - O) k_L a(V) - O \frac{Q_{in}}{V}$$

(3)

The total respiration rate is proportional again to the biodegradation rate, but also considers an offset given by the endogenous respiration rate, $b$. Furthermore, in order to consider limitation due to low DO levels, an additional Monod-type term has been added. It is assumed that the mass transfer coefficient $k_L a$ depends only on the volume if airflow is kept constant.

In this work some simplifications to the model have been made for practicality. The first one assumes that the total biomass $V(t)X(t)$ is constant, since during a single batch cycle its growth is not significant; however, as volume changes, so does its concentration. If $V_0$ is the initial volume and $X_0$ is the initial biomass concentration, then $X(t) = X_0V_0/V(t)$. Therefore, defining $r_{end} = bx_0$ and $D_{in} = Q_{in}/V$, the model for the DO concentration can be re-written as

$$\frac{dO}{dt} = -(r(S_S) + r_{end}) \left(\frac{O}{K_O + O}\right)\lambda(V)$$

$$+ (O_{sat} - O) k_L a(\lambda) - OD_{in}$$

(4)

Under the definition $r^* = \mu^* X_0/Y_{XO}$, the expressions for $r$ and $\lambda$ are

$$r = \frac{r^* S_S S}{S_S S + \alpha(S_S - S)}$$

$$\lambda = \frac{V_0}{V}$$

(5)

The dependence of $k_L a$ on the volume can be assumed linear with respect to $\lambda$, such that

$$k_L a = k_L a_I + (\lambda - \lambda_I) m_{k_L a}$$

(6)

where $k_L a_I$ and $\lambda_I$ are the corresponding values when $V = V_I$. For the substrate concentration it has been convenient to define the quantities $S_S = (Y_{XS}/Y_{XO})S$ and $S_T = (Y_{XS}/Y_{XO})S^*$, whose units are given in the same units as the DO concentration. This yields the following differential equation:

$$\frac{dS_S}{dt} = -r(S_S) \left(\frac{O}{K_O + O}\right)\lambda(V) + (S_{S,in} - S_S)D_{in}$$

(7)

On the other hand, the DO is measured using a sensor whose dynamics may be significant. It has been observed that a linear second order model is appropriate, defined by a time constant, $\tau$:

$$\tau^2 \frac{d^2O_m}{dt^2} + 2\tau \frac{dO_m}{dt} = O - O_m$$

(8)

**Control strategy**

The VTC strategy fills the influent at a fixed flow rate from the initial volume, $V_0$, until the final desired volume, $V_{max}$ (the exchange volume is constant and the filling phase is very fast). The reaction phase is variable in time because it is ended when an exponential DO profile is detected, which happens when substrate has been depleted, because then $r = 0$ and $D_{in} = 0$, and therefore

$$O(t) = O_0 e^{-k_L a t} + \left(O_{sat} - \frac{r_{end}/\lambda_I}{k_L a_I}\right) (1 - e^{-k_L a t})$$

(9)

While this strategy avoids prolonged periods without substrate, thereby hindering deacclimation, it may happen
that the substrate concentration after filling results inhibiting, thus slowing the reaction phase; or even killing the biomass.

As an alternative, the ED-TOC strategy continually measures the DO and using Equation (4) tries to estimate the oxygen mass uptake rate (OMUR), \( \gamma = \frac{(1}{\epsilon} \mu - b)XV \), by differentiating numerically and knowing beforehand the value of critical parameters, e.g. \( k_2 \mu \) and \( O_{sat} \). Since the OMUR is proportional to the specific biomass growth rate, \( \mu \), estimating it on-line allows the use of a control strategy that by turning on and off the fill pumps keeps \( \mu \) near its maximal value, \( \mu^* \); at least until filling up to the maximum volume. Afterwards, the DO profile is monitored as in the VTC strategy in order to determine when to finish the reaction phase (Moreno et al. 2006).

While both strategies have been extensively tested with very good results, including testing in a small scale pilot plant, they suffer from a critical drawback for their practical implementation: the need to constantly measure the DO and rely entirely on a closed loop system which is prone to signal noise, parameter drift, and system faults. On the other hand, the ED-TOC strategy assumes that the measured DO signal, \( O_m \), is close to the DO in the reactor; this assumption may be inconvenient if the sensor dynamics introduce a significant delay that in turn could be worsened by the conditioning filters used to attenuate the signal noise.

The control strategy proposed here takes advantage of the way a SBR operates, so that before the next batch starts, the information gathered from the previous batch is processed and the new operational conditions are set. Of course, this requires continuous on-line measurements of some signals to build up the data base that will be used after the SBR cycle end to perform some calculations, but even if some of the recorded measurements are not trustworthy (e.g. because of sensor malfunction), the outliers can be discarded or the data filtered and thus end up with a useful set of data.

In the case studied here, the reactor operates in batch with only one fill phase and afterwards a reaction phase, but the exchange volume is not constant. Instead, one operational parameter is precisely the exchange volume, \( \Delta V \), such that the final volume is \( V_f = V_0 + \Delta V \). The other operational parameter is the reaction time needed for almost complete mineralization. Assuming that the influent to the reactor does not change significantly from one batch to another, by observing the recently completed batch and estimating model parameters from these observations, the next batch’s operational conditions can be established. If this is repeated batch after batch, the system is able to cope with slowly varying influent characteristics, since it corrects its operation in an adaptive manner. The operational conditions can be programmed into a timer or PLC at the beginning of each batch, rendering the system robust enough to cope with measurement errors, or even faults in the system. If the latter occurs, the PLC keeps the current operational conditions until the fault is corrected. Additionally, some supervision to avoid emergencies can be programmed in closed loop taking advantage of on-line measurements, too.

An optimization criterion is needed for establishing the exchange volume. Since it is not constant and ultimately depends on the substrate concentration in the influent, the total mass of substrate treated may vary. A goal should be to make the SBR operation as efficient as possible and a measure of this is the rate at which mass of substrate in the influent is treated:

\[
B(\Delta V) = \frac{S_{in} \Delta V}{T_{fill} + T_{react} + T_{settle} + T_{draw}}
\]  
(10)

The denominator in the above definition is the total duration of the complete SBR cycle, where each \( T_{xy} \) represents the duration of the corresponding phase. They all depend on \( \Delta V \), the exchange volume: \( T_{fill} = \Delta V/Q_{in} \) and \( T_{draw} = \Delta V/Q_{out} \), while \( T_{settle} \) should be proportional to \( \Delta V \). Under Haldane-type kinetics, \( T_{react} \) depends on how far the value of \( S_m \) is to \( S_m^* \) after filling, which depends on the parameters of the Haldane law, the influent flow rate and the exchange volume. If a model for substrate biodegradation is known (including its parameter values), such as that defined by Equations (1)–(2), then it is possible to perform a numerical optimization to maximize this criterion. The value of \( \Delta V \) to use in the next SBR cycle is chosen as the maximizer to \( B(\Delta V) \). Insofar as the model is adequate enough to describe what has been observed, it does not matter which units are used for the substrate concentration, i.e. the values of \( S_{Sim} \) or \( S_m^* \) are irrelevant as long as the optimization criterion is maximized.

**Parameter estimation**

During the fill and reaction phases the on-line measured DO signal is recorded. With this information the parameters of the model are found such that the error between the measured on-line DO signal, \( S_m \), and that estimated by the model, \( \hat{S}_m \), is minimized in a least squares sense and an *ad-hoc* methodology for parameter estimation is proposed. Before starting the settle or draw phases, a quick test performed by setting the airflow near zero for some time and then to its nominal value for another period allows the estimation of
With the reaction (batch) phase data it is possible now to estimate the parameters of the Haldane law, \( S_{*}, r^{*}, a \), as well as the substrate concentration immediately after filling, \( S_{S,\text{max}} \), by assuming a certain degradation efficiency by the end of this phase. It is also possible to estimate the value of \( O_t = \frac{O_{\text{sat}}}{K_{\text{DO}}} \), since \( k_{La} t \) is assumed constant. With the fill phase data and the obtained parameters so far, the remaining parameters are estimated, \( r_{\text{end}}, O_{\text{sat}}, K_{\text{DO}}, m_{k_{La}}, \) and in order to reach \( S_{S,\text{max}} \) after filling, the value of \( S_{S,\text{m}} \) is finally estimated.

**Experimental strategy**

The pilot reactor was operated as a typical SBR, using both the VTC strategy and the proposed control strategy. The reaction time was the necessary to reach a removal greater than 95% under the known nominal influent substrate concentration. Settle and draw phases were fixed at 20 and 5 min respectively. The reactor was operated for 90 days, where the first 15 days were the period of the acclimation for 4CP biodegradation. During this period the microorganisms were adapted to degrade concentrations of 100, 200 and 250 mg/L of the model compound (4CP) in the influent.

After the acclimation period, the reactor operation was divided in two periods of the same number of days. The first one corresponds to the VTC strategy. Data gathered from these experiments were saved in order to analyse and compare them later. For the second period, the reactor was operated with the proposed strategy, using DO data gathered on the previous cycle to fit a mathematical model and decide the next cycle’s operational conditions. For both periods five sets of synthetic wastewater were prepared, each one of approximately 30 L, which was enough for 13–15 SBR cycles. These were tested subsequently to validate the strategy and its capability of handling varying influent conditions.

**RESULTS AND DISCUSSION**

Figure 1 presents the fit of a representative SBR cycle with respect to the DO concentration, as well as the estimation from simulations of the substrate concentration, \( S_{S} \), and the respiration rate, \( r \). Notice the typical biodegradation profile of the former, as well as the passage of the latter through a maximum twice, first while filling and then while in the batch phase.

The estimation results of some critical model parameters while applying the proposed control strategy on the pilot bioreactor are shown on Table 1. They are divided in the five sets of different preparations of the influent synthetic wastewater. Despite the differences in the means of some values between sets, there is a low variation for each set, which indicates that the parameter estimation algorithm is able to detect the sudden changes in influent characteristics, noticeable on the value of \( S_{m} \), and their influence on the biomass behaviour, manifested in the Haldane law parameters \( a \) and \( r^{*} \). The exchange volume, \( \Delta V \), and the resulting value of the optimization criterion, \( B(\Delta V) \), are also shown.

In order to compare the VTC strategy and the one proposed in this work, for each batch the criterion was also calculated for both of them. The VTC optimization criterion represents the condition that the reactor had been operated with a constant maximal exchange volume, with \( \Delta V_{\text{max}} = 2L \). The percent increase of \( B(\Delta V) \) when comparing these two situations is also presented on Table 1, i.e. \( \%B_{\text{max}} = \frac{B(\Delta V) - B(\Delta V_{\text{max}})}{B(\Delta V_{\text{max}})} \). The evolution of these two criteria is illustrated on Figure 2 for each SBR cycle.
Figure 3, on the other hand, shows the values of $B(\Delta V)$ and $S_{in}$ for each SBR cycle. It is interesting to notice on both of these figures how the changes in the influent concentrations are clearly noticeable for each set of cycles (these are marked on the figures by dashed vertical lines). There are some outliers, especially when there is a sudden change in the influent concentration, but these did not compromise the bioreactor operation.

**CONCLUSIONS**

The proposed control strategy represents an alternative to completely on-line feedback control that copes with slowly varying influent characteristics and their subsequent effect on biomass behaviour. The main advantage of the proposed control paradigm is the post-processing of collected on-line data to set the next cycle’s operational conditions, thereby allowing for elimination of faulty data and thus preventing malfunction of the process during its operation. By first obtaining experimental values for the underlying mathematical model from the previous SBR cycle using the collected dissolved oxygen data and then using the model for optimization, it offers a significant increase in the rate of mass of substrate treated with respect to the performance of a usual SBR operation mode. The results on a pilot bioreactor show the applicability of the strategy, optimizing the rate at which the current mass of substrate in the influent per time unit is treated, setting a priori the exchange volume and the reaction phase duration. Although the proposed strategy was tested for 4-chlorophenol biodegradation in synthetic wastewater, it is applicable to other toxic compounds or even to real wastewater as long as a mathematical model for the biodegradation dynamics that can be parameterized using collected on-line measurements of certain signals is available. Many toxic compounds even in real wastewater exhibit models similar to the one considered in this paper; that is: simple Haldane kinetics. Once the parameters of the model for the previous SBR cycle are determined, the procedure would be exactly the same, i.e. an optimization to maximise the rate at which the mass of influent substrate is being treated.
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REFERENCES