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OPTIMIZATION OF SEQUENCING BATCH (BIO)-REACTORS – CHALLENGING ISSUES

Jérôme HARMAND[a], Denis DOCHAIN[b], Djalel MAZOUNI[a]

[a]*INRA, UR050, Laboratoire de Biotechnologie de l'Environnement, Avenue des Etangs, Narbonne, F-11100, France.*
[b]*CESAME, Université Catholique de Louvain, 4-6 Avenue Georges Lemaître, Louvain-la-Neuve B-1348,, Belgium.*

Abstract: This paper discusses several theoretical as well as practical challenging issues related to a recently developed time-optimal control strategy for the optimization of oxic/anoxic Sequencing Batch Reactors (SBR) for the removal of organic carbon and nitrogen from urban and industrial wastewaters and to its practical implementation. *Copyright © 2007 IFAC*

Keywords: Sequencing Batch Reactors (SBR), mass-balance modeling, automatic control, integrated system, monitoring, optimization, time optimal control.

1. INTRODUCTION

This paper discusses several challenging issues related to a recently developed time-optimal control strategy for the optimization of oxic/anoxic SBRs for the removal of organic carbon and nitrogen from urban and industrial wastewaters and to its practical implementation. While available approaches are essentially numeric or dedicated to very simple reaction networks, restricted to a single reaction such as a carbon removal reaction, (see Moreno, 1999), the actual control law discussed is based on analytical optimization techniques for hybrid systems. It is developed for biological batch systems involving both the carbon and nitrogen removal (in other words, where both anoxic and aerobic conditions must be applied sequentially). The reaction network based on the general mass-balance models principles (see Bastin and Dochain, 1990) considered here is given by :

$$k_1 S_1 \xrightarrow{\varphi_1, Oxygen} X_1$$
$$k_2 S_2 \xrightarrow{\varphi_2, Oxygen} X_2 + k_3 S_3$$
$$k_4 S_1 + k_5 S_3 \xrightarrow{\varphi_3,\ No\ oxygen} X_1$$

where S_1 is the soluble COD[1], S_2 is the ammonium nitrogen concentration and S_3 the skip ammonium while the k_i (i=1…5) are yield coefficients.

Once the system has been modelled under the form of a dynamical model and an optimal control law has been proposed, one may pose the problem of its practical implementation. Because of the lack of relevant information, it appears that the control system could not be applied. It was then proposed to modify the model in order to include the oxygen concentration (which is easy to measure) into the model.

In the first part of the paper, we present the control law and recall its advantages and drawbacks. Then in the second part, we describe the efforts that have been made in order to include the oxygen concentration into the model and the problems encountered when trying to validate a model. It is shown that the model structure is not appropriate to describe the dissolved oxygen dynamics and that additional work is needed to understand the ad/ab-sorption phenomena that appears to exhibit non negligible interferences in the process dynamics.

2. THE TIME-OPTIMAL CONTROL OF A CLASS OF BATCH BIOREACTORS

[1] Chemical Oxygen Demand (a measure of pollution)

2.1 The class of biosystems under interest

Recently a time-optimal control strategy was proposed for the class of batch bioreactor systems described by the following mass-balance models:

Dynamical equations for the aerobic phase

$$\begin{cases} \dot{X}_1 = \mu_1(S_1)X_1 \\ \dot{X}_2 = \mu_2(S_2)X_2 \\ \dot{S}_1 = -k_1\mu_1(S_1)X_1 \\ \dot{S}_2 = -k_2\mu_2(S_2)X_2 \\ \dot{S}_3 = k_3\mu_2(S_2)X_2 \end{cases} \quad (1)$$

Dynamical equations for the anoxic phase

$$\begin{cases} \dot{X}_1 = \mu_3(S_1, S_3)X_1 \\ \dot{X}_2 = 0 \\ \dot{S}_1 = -k_4\mu_3(S_1, S_3)X_1 \\ \dot{S}_2 = 0 \\ \dot{S}_3 = -k_5\mu_3(S_1, S_3)X_1 \end{cases} \quad (2)$$

The kinetics are given by Monod functions $\mu_1 = \mu_{1\max}\frac{S_1}{K_{S1}+S_1}$, $\mu_2 = \mu_{2\max}\frac{S_2}{K_{S2}+S_2}$ and $\mu_3 = \mu_{3\max}\frac{S_1}{K_{S3}+S_1}\frac{S_3}{K_{S4}+S_3}$ where μ_i (i=1..2) are the maximum specific growth rates of the two microorganism consortia and Ks_i (i=1..2) are the corresponding saturation coefficients.

Hypothesis H1: In the above model, oxygen is considered to be a bang-bang control in order to avoid simultaneous nitrification and denitrification activities that were not characterized independently. Thus, oxygen being absent during anoxic phases (no oxygen at all) or saturated during oxic phases (dissolved oxygen concentration>2 mg/l such that the reaction rates are not affected), there was no interest to include it into the dynamical mass-balance equations.

Assuming the input control is the commutation of the aerobic (resp. anoxic) phase to the anoxic (resp. aerobic) phase, it is possible to show that the above systems described by equations (1) and (2) can be reduced to the following third order dynamical system[2]:

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \\ \dot{S}_3 \end{bmatrix} = \begin{bmatrix} f(S_1) \\ g(S_2) \\ -\alpha g(S_2) \end{bmatrix} u + \begin{bmatrix} f(S_1)h(S_3) \\ 0 \\ \beta f(S_1)h(S_3) \end{bmatrix}(1-u) \quad (3)$$

which can be put under the following compact form:

$$\begin{cases} \dot{Z} = F(Z) + G(Z)u \\ Z_0^T = [S_1(0) \quad S_2(0) \quad S_3(0)] \end{cases} \quad (4)$$

where u ($u \in \{0,1\}$, u=0 means that the aeration is off while u=1 means that the aeration is on) is the control variable, Z^T=[S_1, S_2, S_3] and where all functions and parameters depend on the original model equations (1) and (2).

2.2 Control objective and synthesis

For systems that can be put under the form (4), the objective of the control is to compute the switching instants t_1 and t_2 of an aerobic/anoxic/aerobic[3] control sequence (t_1 is the commutation instant from the first aerobic phase to the anoxic phase while t_2 is the commutation instant from the anoxic phase to the second aerobic phase) such that any initial point in the attainable set[4] reaches the target set at t_f (defined as the set of concentrations such that $S_1<S_{1N}$, $S_2<S_{2N}$ and $S_3<S_{3N}$ where S_{1N}, S_{2N} and S_{3N} are normative constraints) in a minimal time t_f- t_0. Assuming that $X_1(t_0)\neq 0$ and $X_2(t_0)\neq 0$, this problem can be mathematically formalized as the search for the two switching instants t_1 and t_2 such that the total reaction time $T=t^1_{aerob}+t_{anox}+t^2_{aerob}$ is minimal. Unless the optimal solution is u=0 (which means that there is almost no ammonium nitrogen (S_2) in the effluent, that is when $S_2(t_0)<S_{2N}$), two distinct cases may arise: either the optimal trajectory first reaches the plane defined by $S_1=S_{1N}$, or the one defined by $S_2=S_{2N}$. Since both concentrations S_1 AND S_2 must comply with $S_1(t_f)<S_{1N}$ AND $S_2(t_f)<S_{2N}$, the problem can be seen as the search for t_1 and t_2 such that:

$$t_{aerobic} = t^1_{aerob} + t^2_{aerob} = \int_{t_0}^{t_1} dt + \int_{t_2}^{tf} dt$$
$$= \max\left(\left(\int_{S_1(t_0)}^{S_1(t_1)} \frac{d\tau}{f(\tau)} + \int_{t_0}^{t_1} \frac{d\tau}{g(\tau)}\right), \left(\int_{S_2(t_0)}^{S_2(t_1)} \frac{d\tau}{f(\tau)} + \int_{S_2(t_2)}^{S_{2N}} \frac{d\tau}{g(\tau)}\right)\right) \quad (5)$$

is minimal (Mazouni *et al*., 2005a). This "max" expression comes precisely from the fact that the optimal trajectory can either first reach the plane defined by $S_1=S_{1N}$, or the one defined by $S_2=S_{2N}$. Taking the max of these times guarantee that both constraints $S_1(t_f)<S_{1N}$ AND $S_2(t_f)<S_{2N}$ are verified.

To solve this general case, the maximum principle was first used to derive necessary optimal conditions. Using this principle, it was shown that there exists a switching plane that defines the commutation instant t_2 while t_1 was computed by introducing a parametrization of the switching instant (see Xu, 2004) and solved numerically using an optimization

[2] Because of the mass conservation, it is possible to transform (1) and (2) into an algebro-differential system (cf. Mazouni et al., 2005b).

[3] It was shown in (Mazouni, 2005a) that any initial point in the attainable set[2] could reach the control target with an aerobic/anoxic/aerobic control sequence.

[4] The attainable set is the set of points for which there exists at least one control sequence, thus defining a trajectory, that drives the initial point towards the final target.

problem corresponding to the search for t_1 that minimizes the anoxic phase time period.

2.3 Discussion and biological interpretation

The biological interpretation of the optimal solution is as follows. The nitrogen removal kinetics is very slow compared to the carbon removal. Thus, the required aerobic time mainly corresponds to the nitrogen removal. The minimal total time needed under oxic conditions is determined by the initial concentration of ammonium nitrogen. Thus the aerobic phase duration cannot be minimized and one can only reduce the total cycle time by reducing the anoxic phase time. In standard cases the anoxic phase takes place at the beginning of the cycle. The anoxic reaction rate depends on both substrate concentrations S_1 and S_3. At the beginning, the maximum of carbon is available. In most cases (depending on the initial conditions), the optimal control strategy consists in starting with an aerobic phase in order to maximize the anoxic reaction rate. During the first aerobic phase, S_3 increases and S_1 decreases. The anoxic phase is applied when the maximal possible rate of the anoxic reaction is reached, so that the total time of this phase is reduced. Of course if the maximum anoxic rate is given at the initial time, the batch starts with the anoxic phase as in the classical approach the total time cannot be further reduced.

3. APPLYING OR NOT THIS STRATEGY: THAT IS THE QUESTION…

As usual, it is possible to apply the previous optimal strategy in open loop: assuming the initial conditions are known, compute the commutation instants and wait for the end of the phase treatment hoping the trajectory actually reaches the target. However, the uncertainty on the model makes this strategy highly questionable in practice. A more appropriate way to apply an optimal control strategy consists in "closing the loop": from the theoretical commutation instants, one generates the corresponding optimal trajectory and tracks this trajectory using the information available on-line through the sensors and commutations between aerobic and anoxic phases as the control input. However, in the present case, all the substrate concentrations (S_1, S_2 and S_3) would be needed for our optimal control strategy to be appropriately applied in closed loop. Although a number of innovative new sensor devices were developed within the EOLI project[5], none of them were able to provide all three required concentrations. Furthermore, the sampling periods of the developed sensors were not short enough to be used within the previously presented control strategy applied in closed loop. An interesting alternative would be to use the dissolved oxygen - which is much easier to measure in practice than other substrates - as a tool for process monitoring and/or as a detector for the commutations between phases. In order to evaluate the performance of the optimal control strategy in connection with the oxygen concentration, it is important to consider a dynamical model that incorporates its dynamics.

[5] European project (2002-2005) dedicated to the optimization of biological Sequencing Batch Reactors.

4. MODELING BATCH OXIC/ANOXIC BIOREACTORS INCLUDING THE DISSOLVED OXYGEN CONCENTRATION

4.1 A modified model for the aerobic phase

The challenging issues discussed in the following are related to the modelling of the aerobic phase. Thus, we restrict our attention to this phase in what follows. The general model to be developed is given by:

$$\begin{cases} \dot{X}_1 = \mu_1(S_1, S_4)X_1 \\ \dot{X}_2 = \mu_2(S_2, S_4)X_2 \\ \dot{S}_1 = -k_1\mu_1(S_1, S_4)X_1 \\ \dot{S}_2 = -k_2\mu_2(S_2, S_4)X_2 \\ \dot{S}_3 = k_3\mu_2(S_2, S_4)X_2 \\ \dot{S}_4 = k_L a\left(S_4^* - S_4\right) - k_4\mu_1(S_1, S_4)X_1 - k_5\mu_2(S_2, S_4)X_2 \end{cases} \quad (6)$$

where $\mu_1 = \mu_{1\max}\dfrac{S_1}{K_{S1}+S_1}\dfrac{S_4}{K_{O1}+S_4}$, $\mu_2 = \mu_{2\max}\dfrac{S_2}{K_{S2}+S_2}\dfrac{S_4}{K_{O2}+S_4}$, S_4 is the oxygen concentration, S_4^* is the oxygen saturation concentration, k_La is the oxygen transfer coefficient while k_1 and k_5 are yield coefficients.

For the sake of simplicity, this model will be denoted by "model #1" in what follows. The details of both the experiments and the identification procedures are not presented here because of lack of space. We only present here below the identification results (they are based on twelve experiments that were realized following an experimental planning involving different input loads and input air flow rates).

Table 1: Identification results for the model #1

$\mu_{1\max}$	$5.9\times10^{-3}\pm7\times10^{-4}$ (1/T)
Ks_1	$1.55\pm2.08\times10^{-1}$ (M/L)
K_{O1}	$1\times10^{-5}\pm1\times10^{-6}$ (M/L)
$\mu_{2\max}$	$2.16\times10^{-2}\pm4.24\times10^{-3}$ (1/T)
Ks_2	$2.40\times10^{-1}\pm5.31\times10^{-2}$ (M/L)
K_{O2}	$2.16\times10^{-2}\pm4.4\times10^{-3}$ (M/L)
$1/k_1$	1.49±0.53 (M/M)
$1/k_2$	0.80±0.20 (M/M)
k_3/k_2	0.50±0.14 (M/M)
k_4	$8.57\times10^{-1}\pm5.01\times10^{-2}$ (M/M)
k_5	$3.42\pm3.07\times10^{-1}$ (M/M)

Regarding the very good affinity of the biomass X_1 with respect to both S_1 (see figures 1 to 3) and S_4 (very low values of Ks_1 and K_{O1} with respect to the orders of magnitude of S_1 and S_4, cf. Table 1), it is

possible to replace the growth function μ_1 by $\mu_{1\max}S_1$. A similar line of reasoning allows to modify μ_2 in a similar way. The new model structure obtained using the above simplifications is called model #2. Now, it can be observed that the biomass concentrations are almost constant during one treatment cycle. In more precise terms, one can say that the change in biomass concentrations is not significant with respect to the measurement accuracy used for characterizing them.

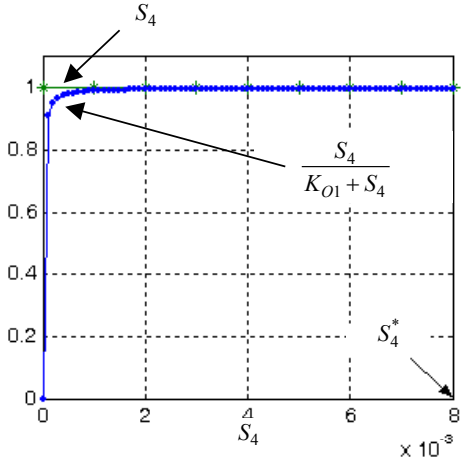

Figure 1: Oxygen (S_4) Monod kinetics identified within the model #1 and approximation with a constant

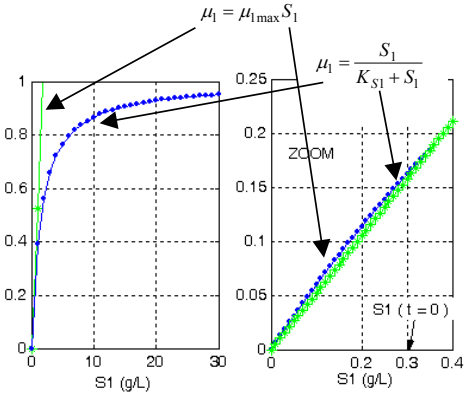

Figure 2: Carbon (S_1) Monod kinetics identified within the model #1 and its linear approximation

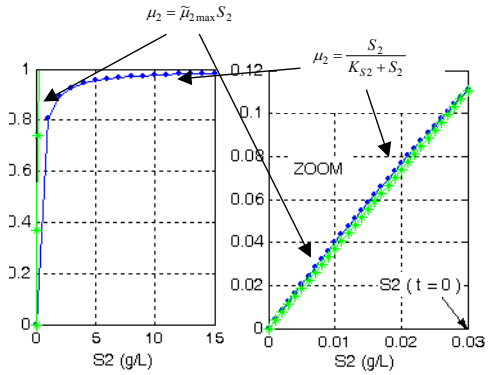

Figure 3: Nitrogen (S_2) Monod kinetics identified within the model #1 and its linear approximation

Thus, over a given cycle, they can be considered as constant leading to a third model – completely linear - denoted model #3 and involving only four states S_1, S_2, S_3 and S_4 as:

$$\begin{cases} \dot{S}_1 = -k_1\mu_{1\max}S_1 \\ \dot{S}_2 = -k_2\mu_{2\max}S_2 \\ \dot{S}_3 = k_3\mu_{2\max}S_2 \\ \dot{S}_4 = k_L a\left(S_4^* - S_4\right) - k_4\mu_{1\max}S_1 - k_5\mu_{2\max}S_2 \end{cases}$$

Where the parameters are given in the Table 2:

Table 2: Identification results for the model #3

$\mu_{1\max}$	$2.66\times10^{-2}\pm4\times10^{-4}$ (1/T)
$\mu_{2\max}$	$4.20\times10^{-3}\pm0.8\times10^{-4}$ (1/T)
k_4	$4.99\pm2.553\times10^{-1}$ (M/M)
k_5	$2.03\pm2.78\times10^{-1}$ (M/M)

the other parameters being unchanged.

Comparisons between some data and models #1, #2 and #3 are shown in figures 4.

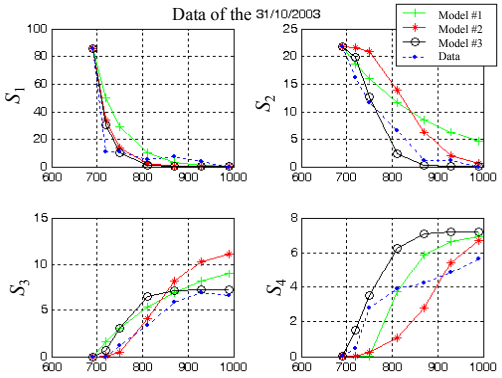

Figure 4: Comparisons between one data set and models #1, #2 and #3

4.2 Discussion and open problems

The modelling results presented hereabove illustrates several problems.

First the fact that a linear model can capture – almost without loss of accuracy when compared to a nonlinear model – the dynamics of the substrate is a priori quite surprising. It can indeed be easily explained when carefully looking at the experiments. For the biomasses, as explained above, it should be noticed that microorganisms concentrations remain almost constant over one phase cycle. For the substrates, it depends indeed on the applied load. The linear behaviour is directly related to the local rate of the kinetics. Even if the substrate concentrations were high (the reaction kinetics are then saturated), the consequence would simply be a delay in the substrate dynamics – quite small in regard to the high biomass concentrations that were used during the experiments.

Secondly it should be noticed that from the modelling point of view, the results are not satisfying regarding the modelling of oxygen dynamics. The simplifications that have been made on the kinetics

of the substrates (oxygen does no longer appear in the kinetics) show that the experiments were indeed realized under conditions where the oxygen concentration were not interfering with the substrate dynamics. However, even under these conditions and, in fact, in any case, the last equation of the set of equations (7) (the differential equation describing the oxygen dynamics) should have been able to capture the oxygen dynamics. Obviously, there is an intrinsic problem in the model structure that would need to be understood. We shall come back on this issue later on.

Thirdly, from a control point of view, it should be noted that modifying the model usually leads to the impossibility of applying the original optimal control law. In fact, here, it is not really a problem. Indeed, the most important assumption is that the oxygen is non-limiting under aerobic conditions. As a consequence, if the oxygen is kept constant (for instance by a local control loop acting on the air flow), then the oxygen concentration in the kinetics enters into the maximum growth rate constants $\mu_{i\max}$ (i=1,2) and nothing changes with respect to the control strategy proposed in section 2. However, the objective when introducing the oxygen within the model is to modify the control objective, that is to modify the optimization criterion. One open problem would be to solve an energy-optimal control problem and (why not?) a mixed problem where one could weight the time-optimal versus the energy-optimal control problems as follows:

$$J = \int_{t_0}^{t_f} d\tau + \lambda \int_{t_0}^{t_f} S_4^2(\tau) d\tau \qquad (7)$$

However, such an optimization problem would really be of interest if the model developed is such that it allows simultaneous nitrification/denitrification phenomena. In other terms, the optimization problems should now be solved for the following class of models:

$$\begin{cases} \dot{X}_1 = \mu_1(S_1,S_4)X_1 + \mu_3(S_1,S_3,S_4)X_1 \\ \dot{X}_2 = \mu_2(S_2,S_4)X_2 \\ \dot{S}_1 = -k_1\mu_1(S_1,S_4)X_1 - k_2\mu_3(S_1,S_3,S_4)X_1 \\ \dot{S}_2 = -k_3\mu_2(S_2,S_4)X_2 \\ \dot{S}_3 = k_4\mu_2(S_2,S_4)X_2 - k_5\mu_3(S_1,S_3,S_4)X_1 \\ \dot{S}_4 = k_L a(S_4^* - S_4) - k_6\mu_1(S_1,S_4)X_1 - k_7\mu_2(S_2,S_4)X_2 \end{cases}$$

which captures all the biological reactions occurring in the aerobic as well as the anoxic phases, and where $\mu_1 = \mu_{1\max}\frac{S_1}{K_{S1}+S_1}\frac{S_4}{K_{O1}+S_4}$, $\mu_2 = \mu_{2\max}\frac{S_2}{K_{S2}+S_2}\frac{S_4}{K_{O2}+S_4}$ and $\mu_3 = \mu_{3\max}\frac{S_1}{K_{S3}+S_1}\frac{S_3}{K_{S4}+S_3}\frac{K_{O3}}{K_{O3}+S_4}$.

In a first attempt, S_4 could be considered as the control input such that the system can be reduced to only five variables while in a second step, k_La could be considered as the control. Another remark in a first attempt is that the switching function in μ_3 could be taken as the counterpart of $S_4/(K_{O2}+S_4)$, that is :

$$\mu_3 = \mu_{3\max}\frac{S_1}{K_{S3}+S_1}\frac{S_3}{K_{S4}+S_3}\frac{K_{O2}}{K_{O2}+S_4}.$$

4.3 The role of ad/ab-sorption

Let us now go back to the problem of modelling the oxygen concentration. From figure 4, it seems that model 3 overestimates the dissolved oxygen. The hypothesis we formulate here to explain such a model behaviour is related to ad/ab-sorption phenomena. Indeed, there is a number of experimental data that support this assertion. For instance, in the data set of October 31, 2003 used for model validation (cf. figure 4), the theoretical initial values for the degradable carbon (S_1) was 140 mg/l while that of the organic nitrogen was theoretically of 30 mg/l instead of 80 and 25 mg/l, respectively. Assuming that the easily (or even low) degradable COD or nitrogen is ad/ab-sorbed just after inoculation could explain the oxygen consumed is underestimated by the model. If an important part of the COD is ad/ab-sorbed, then some oxygen is indeed consumed to degrade it and nothing can be observed in the liquid phase. A number of experiments were realized in order to estimate the quantity of COD/nitrogen ad/ab-sorbed by biomass mass unit at the initial stage of the reaction phase.

These phenomena could be included in the model. To do so, an experimental protocol was defined :

1) characterization of the CAC[6] dependence with COD concentration per unit sludge mass,
2) determination of the CAC variation from an influent to another.

The experiments were performed in an one litre batch reactor where conditions were such that it can be assumed that the COD concentration reduction is due only to the ad/ab-sorption phenomena. Figure 5 shows the evolution of the COD concentration during the time in the batches. Due to the CAC, the COD decreases very quickly and then reaches a steady value because there is no biological removal. Additional experiments were dedicated to determine the relationships between the ad/ab-sorbed COD and the initial concentration of the influent. Since our objective is to characterize the CAC per unit sludge mass, COD concentration was divided per the TSS[7] concentration witch was equal to 3 g/l.

[6] COD Ad/ab-sorption Capacity
[7] Total Suspended Solids

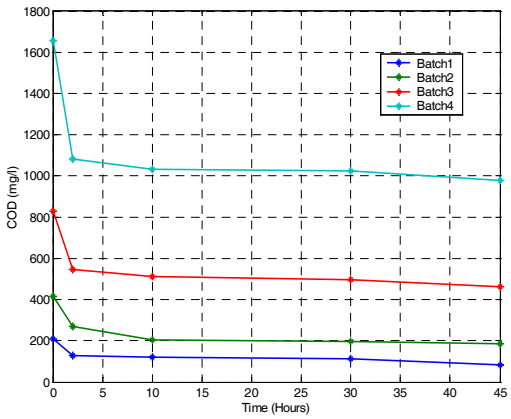

Figure 5 : COD reduction in closed batch reactor without aeration

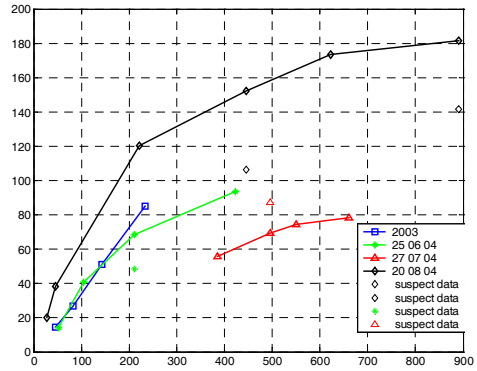

Figure 6 : Evolution of the characteristics of the CAC (data shown are raw data : "suspect data" means probable outliers)

The results are shown in Figure 6 for a constant COD concentration. The different colours correspond to identical experiments realized at constant intervals of one month. Obviously, the CAC by gram of TSS varies in time. In other words, either the sludge or the influent characteristics have changed. To investigate these changes, a third series of experiments were realized in changing the carbon sources. As expected, the CAC varied with influent characteristics : no ad/ab-sorption was observed with acetate while initial ad/ab-soprtion was noticed with whey and lactose (results not shown).

These experimental data allowed us to conclude that :

- the underestimated quantity of oxygen consumed can be explained by ad/ab-sorption phenomena,
- the CAC obviously depends on both the sludge and influent concentration and, as a consequence,
- the CAC varies over the time…

These results make the introduction of a new ad/ab-sorption compartment into the model quite questionable. It is not realistic from a practical point of view to ask technician to characterize both the sludge and influent characteristics before testing the model. Thus, it was not possible to systematically characterize this phenomenon and more work is needed to address and quantify our hypothesis.

5. CONCLUSIONS AND PERSPECTIVES

In this paper, optimal control of oxic/anoxic sequencing batch bioreactors has been discussed. On the basis of a simple mechanistic model and under the assumption that no simultaneous nitrification/denitrification occurs, we have first presented a new time-optimal control strategy. One of the most interesting result of this control law is that in a number of cases, it suggests to add a small aerobic period at the beginning of the treatment cycle while it is not usually the case in practice. In a second part, the difficulties of applying such a control law in practice have been pointed out. In particular, it was suggested that the dissolved oxygen concentration which is not included in the model could be used as a monitoring tool within this control strategy. A model structure including this new variable was proposed together with identification results. It was then pointed out that the new structure which complies with the mass-balance principle was not able to appropriately capture the dissolved oxygen dynamics suggesting that this new model needed to be improved. A number of challenging issues were then suggested while the possible interfering role of ad/ab-sorption phenomena was underlined.

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