A SIMPLE MASS BALANCE MODEL FOR BIOLOGICAL SEQUENCING BATCH REACTORS USED FOR CARBON AND NITROGEN REMOVAL

D.Mazouni[1], M. Ignatova[2], J. Harmand[1],

[1]*Laboratoire de Biotechnologie de l'Environnement,Institut National de la Recherche Agronomique,*
Avenue des étangs, 11100 Narbonne, France.
mazouni@ensam.inra.fr, fax : (+33) 468.425.160,tel : (+33) 468.425.159
[2]*Institute of Control and System Research, Bulgarian Academy of Sciences*
P.O.Box 79, 1113 Sofia Bulgaria
ignatova@icsr.bas.bg, fax +00359 2 870.33.61, tel. +00359 2.979.20.52)

Abstract: This paper presents a very simple mass balance model structure for Sequencing Batch Reactors used for the biological treatment of organic carbon and nitrogen. This model is intended to be used for control purposes. As such, the degree of details required is not too high and only major biological processes are taken into account. This model is identified and validated with real data acquired on a real SBR pilot plant. Some conclusions and perspectives are then drawn. *Copyright@2004 IFAC*

Keywords: Sequencing Batch Reactors (SBR), biological treatment, modelling, parameter identification

1.INTRODUCTION

Increasing requirement of nitrogen and carbon removal has led to the development of the activated sludge Sequencing Batch Reactor (SBR). The SBR is a reliable and low cost treatment process. But most importantly, its advantages are related to its ability to easily deal with sludge settlement which is difficult to maintain in good conditions in classical activated sludge processes due to the persistent incoming hydraulic shock loads

The SBR process is characterized by a series of process phases : fill, react, settle and draw. All of them take place in the same tank. Initially, the reactor contains a volume V_o and a quantity of biomass X_o that remains from the last cycle. The cycle starts by introducing a volume $\nabla V = V_{max} - V_{min}$ into the reactor with a flow rate Q. The reaction phase can be divided in two sub-phases : aerated and non-aerated. These two steps allow both carbon and nitrogen removal. During these phases the reactor is maintained perfectly homogeneous. Once the reaction phase is completed, the agitation is stopped and the

sludge starts flocculating and settling. The clean supernatant is then separated from the sludge and can be withdrawn from the reactor. The reactor is then available to receive a new volume ∇V of wastewater. After few cycles, because the pollution is transformed into biomass, it is necessary to waste some sludge (Wilderer and al., 2001).

A detailed Activated Sludge Model (ASM1) was presented in (Jeppsson, 1996; Henze and al., 1987) by the IAWQ Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment Processes. The process dynamics incorporate not only major phenomena such as carbon oxidation, nitrification and denitrification, but also decay of biomass due to mortality, hydrolysis of biomass and so on leading to a quite complex model involving not less than 13 variables and about 20 parameters. Although largely used over these last 15 years, it should be emphasized that such complex models are not suited for control purposes. Instead, a reduced and simple model for control design and optimisation of SBR activated sludge processes is proposed in this paper. To do so, a general method for

modelling bioreactors from the reaction scheme is applied (Bastin and al., 1990; Dochain and al., 2001). This method is based on the mass balances in the reactor and only takes into account the three more important biological phenomena: aerobic carbon and ammonium nitrogen oxydation and anoxic carbon and nitrate denitrification. The concentrations of all organic materials including biomass are in Chemical Oxygen Demand (COD) units. The COD measure provides a link between electron equivalent in the organic substrate, the biomass and the oxygen utilized. Futhermore, mass balances can be made in terms of COD.

The proposed model is identified and cross-validated using 15 experiments that were carried out from 05.08.2003 to 15.04.2004 in the Laboratory of Environmental Biotechnology (LBE) INRA Narbonne, France. More specifically, eight experiments are used for parameter identification while 7 are used for model verification. Finally, some conclusions and perspectives are drawn.

2.MATERIALS AND METHODS

2.1 Reactor design and start up phase

Activated sludge:
The sludge used in the LBE SBR comes from the urban wastewater treatment plant of COURSAN, south of France. This plant was chosen because both carbon and nitrogen are treated in aerobic and anoxic conditions. The tank was filled with about 100 litters of this sludge. For two month, the sludge was simply aerated and filled with a low organic loading rate (<0.7 kg COD/m^3/day). After three months of start up, the purification rate was around 98% and a high sludge settleability with no suspended solid after decant was obtained.

Influent wastewater
Semi-synthetic dairy wastewater is used as influent. This fed is prepared by dilution of concentrated whey collected in a cheese dairy. The characteristics of the whey correspond to 70 g/L of COD and 2 g/L of total kjedahl nitrogen (NTK). In order to change the C/N ratio of the whey, organic nitrogen as Urea (CH_4N_2O) is added.

The whey is maintained at –20°C in small bottles. About 3.6 litres are used per day to prepare reactor's feed. In standard conditions, the influent volume treated after dilution is 50 l/day. Its average composition is : 5 g/L COD, 250 mg/L N-NTK, *and pH = 6,23.

Pilot plant
The tank of the reactor has a cylindrical form. Its dimensions are 50cm ∅ and 130cm height with a total volume of 255L. It is equipped with a variable flow rate pump to fill the reactor and a controlled valve to withdraw the effluent and the sludge in

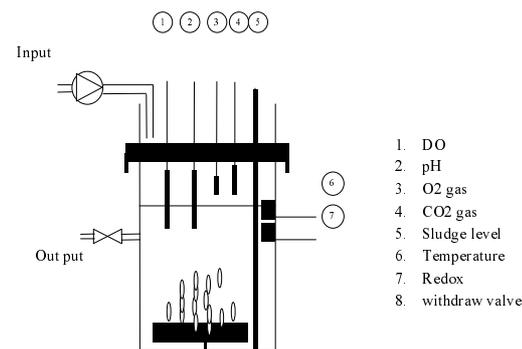excess. Air is used for aeration and mixing. Its flow is controlled by a flow meter.

1.	DO
2.	pH
3.	O2 gas
4.	CO2 gas
5.	Sludge level
6.	Temperature
7.	Redox
8.	withdraw valve

Fig 1 : SBR pilot plant

The reactor is operated at an ambient lab temperature of 20°C. Each cycle duration is 24 hours. More specifically, the reaction phases are divided into 2 periods. In each one, half of the total influent daily volume is added (25 liters). A schematic view of the operating modes is shown in Fig. 2.
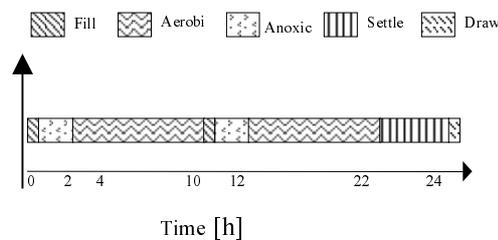
Fig.2 Cycle phases

2.2 Measurements

On line data
The following parameters are available on line : pH, Redox, Temperature, Dissolved Oxygen (DO), CO2 gas, O2 gas, sludge blanket, influent air flow rate and input air flow rate.

All sensors and actuators are connected to a PC and the functioning of the process is completely automated. The on-line measurements are captured by an home-made software called Modular Serial buffer Process Control (MSPC) and stored in a database. Matlab is used to control the reactor via MSPC.

Off line data:
The off line measurements are : COD (total and soluble), NTK, Nitrite, Nitrate, Ammonium, TSS and VSS. For all these measurements, standard methods are used.

3. MODELLING

A biological reactor with microorganisms able to perform carbon and nitrogen removal under adequate conditions of temperature, pH, is considered.

Let us define the following notations for the concentrations :

X_1 : Heterotrophic microorganisms. (mg/l)
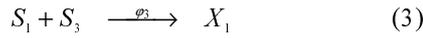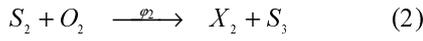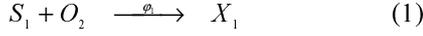X_2 : Autotrophic microorganisms (mg/l)
S_1 : Organic carbon. (mg COD /l)
S_2 : Ammonium nitrogen. (mg N-NH4/l)
S_3 : Nitrates/Nitrites nitrogen (mg N-NO3/l+ mg N-NO2/l)
O_2: Dissolved oxygen (mg O2/l)

The reaction network is given by:

$$S_1 + O_2 \xrightarrow{\varphi_1} X_1 \tag{1}$$

$$S_2 + O_2 \xrightarrow{\varphi_2} X_2 + S_3 \tag{2}$$

$$S_1 + S_3 \xrightarrow{\varphi_3} X_1 \tag{3}$$

In the wastewater, nitrogen is essentially under organic form. It is rapidly ammonified into NH_4^+. During the biological reactions the ammonium is transformed into nitrogen gas N_2 in two steps: nitrification and denitrification (Jeppsson, 1996; Henze and al., 1987). Nitrification is realized by Autotrophic bacteria under aerobic conditions (reaction 2). It is a two step reaction : nitritation where ammonium is converted into nitrites NO_2^- and nitratation where nitrites are converted into nitrates NO_3^-. In order to simplify the model, these two reactions are usually grouped together in one reaction where ammonium is directly converted into nitrates by Autotrophic bacteria X_2 with the growth rate $\varphi_2(.)$.

Denitrification is reducing nitrates into nitrogen gas. This reaction is done by Heterotrophic bacteria under anoxic conditions (presence of NO_3^-, absence of O_2). This bacteria uses nitrites as electron acceptor when no oxygen is available. This reaction only takes place if organic carbon is available. In anoxic condition the heterothrophic growth rate is given by $\varphi_3(.)$.

Carbon removal is realized by Heterotrophic bacteria (Henze and al., 1987). Carbon can be eliminated either under anoxic conditions with nitrates in denitrification phase (reaction 3) or under aerobic conditions (reaction 1). In the last case, the growth rate of Heterotrophic is $\varphi_1(.)$. In order to have the three reactions in the same tank, we should consider two sub-phases reactions : aerobic sub-phase to nitrify the nitrogen and an anoxic sub-phase to denitrify it. The carbon is eliminated in both cases.

In this section, a general state space model for the description of SBR activated sludge process is proposed. The modelling is based on the mass balance in the reactor during the two phases anoxic and aerobic. What can happen biologically during the settling phase is neglected. Considering the reaction scheme (1 to 3), we can apply the mass balance principle to determine the state space model for both anoxic and aerobic phases.

Aerobic model :

$$\frac{dX_1}{dt} = \mu_1(S_1, O_2)X_1 \tag{4}$$

$$\frac{dX_2}{dt} = \mu_2(S_2, O_2)X_2 \tag{5}$$

$$\frac{dS_1}{dt} = -k_{11}\mu_1(S_1, O_2)X_1 \tag{6}$$

$$\frac{dS_2}{dt} = -k_{22}\mu_2(S_2, O_2)X_2 \tag{7}$$

$$\frac{dS_3}{dt} = k_{32}\mu_2(S_2, O_2)X_2 \tag{8}$$

Anoxic model :

$$\frac{dX_1}{dt} = \mu_3(S_1, S_3)X_1 \tag{9}$$

$$\frac{dS_1}{dt} = -k_{13}\mu_3(S_1, S_3)X_1 \tag{10}$$

$$\frac{dS_3}{dt} = -k_{33}\mu_3(S_1, S_3)X_1 \tag{11}$$

with

$$\mu_1 = \mu_{1\max}\frac{S_1}{K_{S1} + S_1}O_2;$$

$$\mu_2 = \mu_{2\max}\frac{S_2}{K_{S2} + S_2}O_2; \tag{12}$$

$$\mu_3 = \mu_{3\max}\frac{S_3}{K_{S3} + S_3}\frac{S_1}{K_{S1} + S_1} \tag{13}$$

As can be seen, the specific growth rates in aerobic phase, μ_1 and μ_2, are proportional to the dissolved oxygen concentration, O_2, in the reactor instead of the classical expression $\dfrac{O_2}{K_O + O_2}$ proposed in (Henze and al., 1987). It is essentially because the available experiments were realized with a non-limiting oxygen concentration. Furthermore, to avoid identification problems involving oxygen transfer coefficient, the O_2 is considered as an input variable for model parameter identification.

4. MODEL IDENTIFICATION

The price to pay to this oversimplification of the model is that the models obtained are only valid for a small period of time and under specific aeration conditions. If the input air flow rate is changed or if the sludge characteristics significantly change, the model should be re-identified. As explained before, two sub-models are considered - one for the aerobic phase and another for the anoxic phase. The identification of the model parameters is made separately for each available data sets, (#4–#8 & #12) and (#9–#11 & #13). Each data set corresponds to one SBR cycle where the influent concentrations were changed as it is mentioned in Table 1.

Table 1 Influent concentration and air flow rate for each experimental data used for identification

Exp. N	Air flow (l/min)	COD in (mg/l)	NTK in (mg/l)
26.06.03	30	3026,09	252
05.08.03	30	1980,84	173,6
27.10.03	50	4318,18	168,00
29.10.03	50	4772,25	183,68
31.10.03	50	4476,92	204,40
04.11.03	50	4836,85	319,20
06.11.03	75	4235,45	260,4
12.11.03	25	4945,61	285,60

A smart optimization algorithm was used for this purpose. The algorithm folder consists of four programs. They are shown in the Fig. 3. Main program (*main.m*) functions are used :
- to plot experimental and model simulation data ;
- to define list and initial values of model parameters to be estimated
- for the smart estimation procedure.

The smart estimation procedure is a simple algorithm. The criterion to be minimized was chosen to be the Sum of Square Error (SSE). To escape a program stop in cases of a big error at the beginning of the procedure, the initial value of "smallest_error" can be set big enough. On the next step, the real value of error is accepted as "smallest_error". Furthermore, a local minimum of the criteria function could be escaped by changing the algorithm parameter named Previously Set Number (PSN). On each step of optimization procedure, the "smallest_error" is updated with a random vector that is multiplied by that PSN.
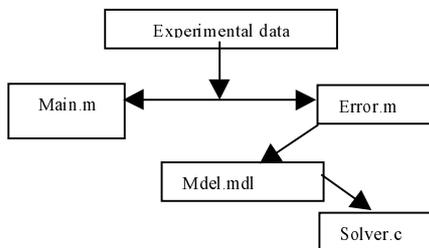

Fig. 3 Relationship of identification algorithm programms

The program *error.m* defines values of :
- constants;
- initial values of model variables
-    calculation of criteria SSE.

The programs *model.mdl* and *solver.c* invoke a S-function for solving the differential equations of the process model

5. RESULTS AND DISCUSSION

Eight experiments are chosen for parameter identification of both process models. The experiments were carried out in two different periods of the year : summer experiments (26.06.2003 and

05.08.2003) and winter experiments (three experiments in October, and three in November). The aerobic model, (#4–#8 & #12) consists of five variable and seven parameters. The parameters μ_{1max}, μ_{2max} are the maximum specific growth rates of Heterotrophic and Autotrophic microorganisms respectively; K_{S1}, K_{S2} are saturation constants associated with substrates S_1 and S_2 respectively; k_{11}, k_{12} and k_{32} are the yield coefficients for degradation of S_1 by X_1 and S_2 by X_2 ; and for production of S_3 by X_2 respectively.

The results of the aerobic model of the parameter identification are shown in Table 2.

Table 2 Estimated parameters for aerobic model

Exp. N	μ_{1max}	μ_{2max}	K_{S1}	K_{S2}	k_{11}	k_{22}	k_{32}
26.06.03	0.0223	0.0074	26.6083	130.1183	3.0062	2.03450	0.7303
05.08.03	0.0260	0.0119	24.0943	86.1134	3.1019	1.2067	2.0998
27.10.03	0.0123	0.0056	38.8450	150.8545	1.6281	2.2202	0.6674
29.10.03	0.0125	0.0053	35.9126	153.7505	1.5129	2.1062	0.6317
31.10.03	0.0172	0.0057	28.9683	141.8389	2.4329	2.2770	0.6457
04.11.03	0.0113	0.0068	40.1694	127.6472	1.8928	2.2637	0.6810
06.11.03	0.0157	0.0059	25.7763	149.4329	2.4549	2.0903	0.5902
12.11.03	0.0239	0.0064	26.8919	150.1729	3.3777	2.1598	0.6312

The anoxic model, (#9–#11 & #13). consists of tree variables and five parameters. The parameter μ_{3max} is maximum specific growth rate of Heterotrophic microorganisms for anoxic phase; K_{S3} is the saturation constant associated with substrate S_3 ; k_{33} and k_{13} are yield coefficients for the degradation of S_1 and S_3 by X_1 respectively.

The results of the aerobic model the parameter identification are shown in Table 3 :

Table 3 Estimated parameters for anoxic model

Exp No	μ_{3max}	K_{S1}	K_{S3}	K_{33}	K_{13}
26.06.03	0.4871	20.3854	30.2249	0.2496	6.6738
05.08.03	0.4283	26.9341	22.3217	0.2439	7.0829
27.10.03	0.2732	15.2957	36.0271	0.0842	11.9000
29.10.03	0.4675	22.7470	17.7671	0.2844	13.0682
31.10.03	0.7069	32.7058	18.6532	0.1994	15.7103
04.11.03	0.6099	29.8587	12.3886	0.2282	18.2023
06.11.03	0.5586	27.6960	15.4761	0.1800	17.5179
12.11.03	0.3542	38.0821	21.7736	0.1045	13.6391

The model was validated by comparing the model simulation curves with experimental data. In Figures.4 and 5, the values of model parameters taken from the corresponding rows of Tables 2 and 3 respectively are used for model simulation.

In Figures 6 and 7, medium values for each parameter is used for both models simulations. The models are cross validated with data of the new experiments (06.04.04 and 15.04.04), that are not listed in Tables 2 and 3.
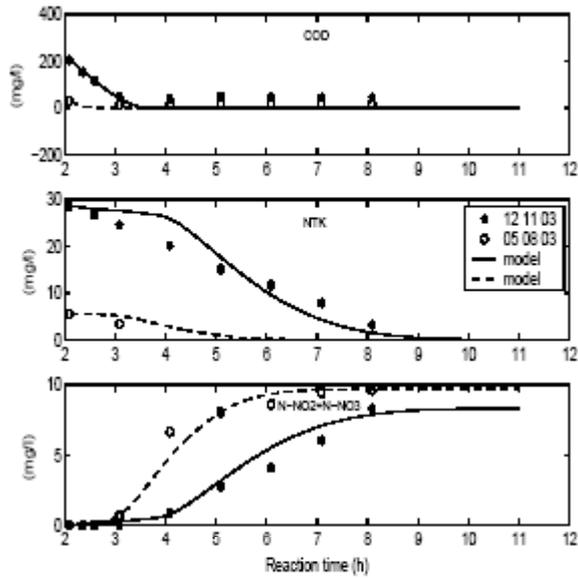
Fig. 4 Aerobic model verification

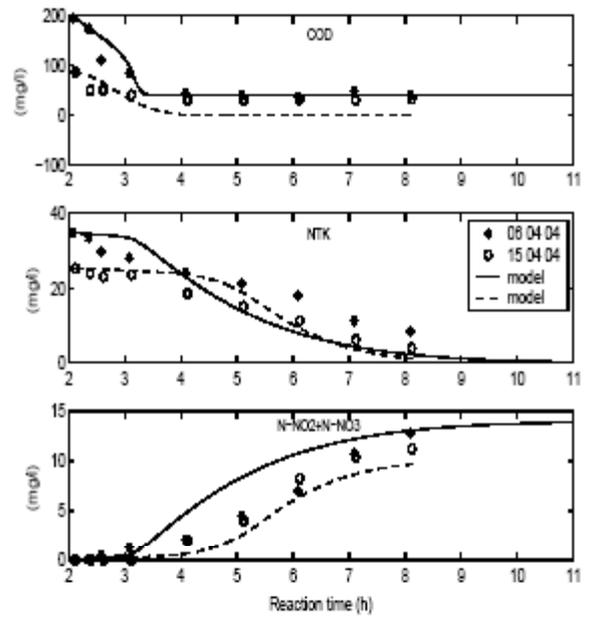where S* is the average of residual COD in the reactor.
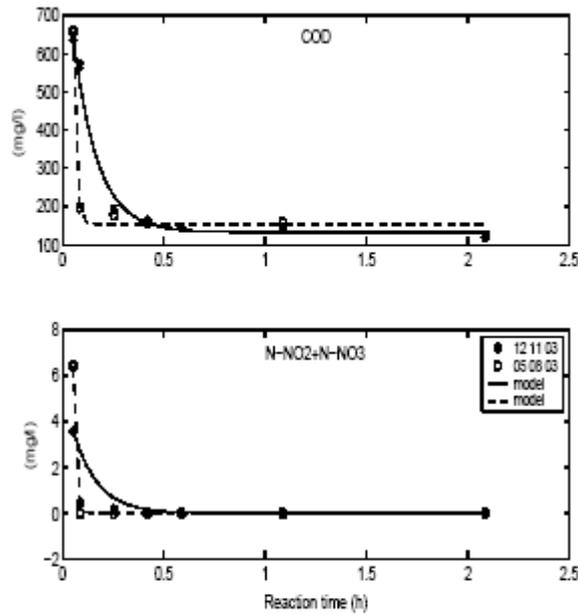

Fig. 6 Aerobic model verification
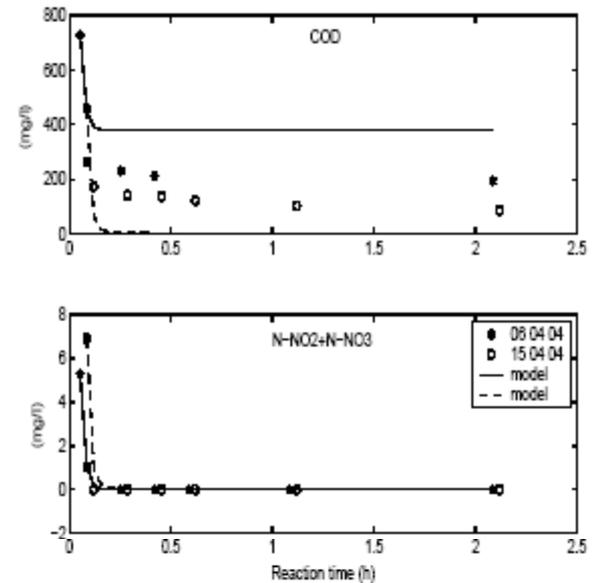

Fig. 5 Anoxic model verification

Fig. 7 Anoxic model verification

At the end of the aerobic phase, a static error between the model and the COD measurements is observed in Fig. 6. This variation is related to the non biodegradable COD in the wastewater and the slowly biodegradable COD generated by biomass decay (Orhoni and al., 2003). This residual COD is a constant value and it is around 40 mg/l. To adapt the model, we propose the modified growth rate function $\mu_1^{'}$.

$$\mu_1^{'} = \mu_{1max} \frac{S_1 - S_1^{*}}{K_{S1} + (S_1 - S_1^{*})} O_2 \qquad (14)$$

The experiments were performed in three periods of the year: Jun-July 2003, November-October 2003 and Mars-April 2004. Data of the experiments carried out 2004 are used for model validation only.

For a small period, the model is robust and its parameters are valid for a variation of 50% of substrate concentration. However, these parameters vary during the year because of the variation of the dairy effluent composition from season to another, the climatic variations (temperature and pressure…) and the microbial ecosystem variation. Thus the model have to be adapted from time to time with

respect to the variations of the standard conditions and the operating mode of the SBR.

In the anoxic phase, the initial concentration is computed by a dilution factor. We observe a high COD elimination between the initial concentration and the first measured point at T0+2min. If we compare the experiments, we observe that this variation is not related to the nitrate consumption (Kargi and al., 2003; Sozen and al., 1998). i.e the COD/N-Nox ratio for denitrification is not constant. This can be explained by a possible ab(ad)sorption phenomena: a part of COD is used with nitrate nitrogen for denitrification and the other part is stored in the flocks and consumed in the aerobic phase (Krishna and al., 1999). To improve the identification of the anoxic phase a supplementary work will be performed to quantify the part of COD stored according to the biomass concentration and the effluent composition.
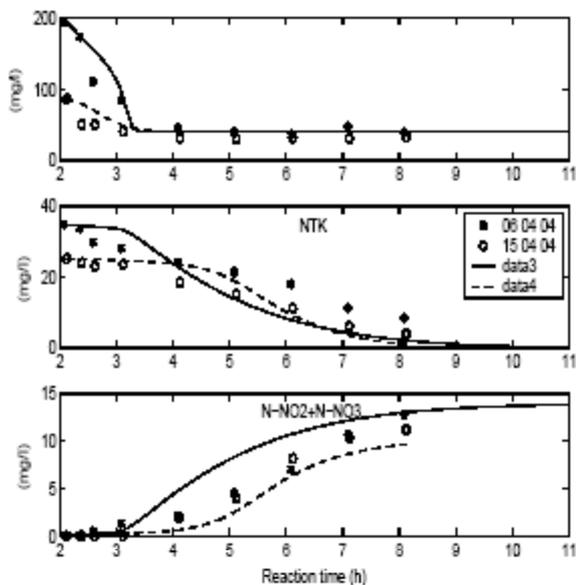

Fig. 8 Aerobic model verification with μ_1 of equation (14)

6. CONCLUSIONS

A very simple mass balance model for Sequencing Batch Reactors used for the biological treatment of organic carbon and nitrogen is presented in the paper. This model is intended to be used for control purposes. As such, the degree of details required is not too high and only major biological processes are taken into account. This model is identified and validated with real data acquired on a SBR pilot plant operating in the LBE, Narbonne, France. The experiments were performed in three periods of the year: Jun-July 2003, November-October 2003 and Mars-April 2004. Eight experiments are used for model parameter identification. Data of 7 other experiments are used for model validation. A modified growth function is proposed to be investigated as perspectives to adapt the model and

to avoid the static error between the model and the COD measurements at the end of the aerobic phase.

7. ACKNOWLEDGEMENT

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