10th International IFAC Symposium on
Computer Applications in Biotechnology
Preprints Vol.2, June 4-6, 2007, Cancún, Mexico

IMPLEMENTATION OF TOXIC INHIBITION IN WASTEWATER TREATMENT PLANT BENCHMARK SIMULATION MODELS

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Abstract: The activated sludge process of wastewater treatment plant benchmark simulation models has been modified to include the effect of soluble, biodegradable or non biodegradable toxic substances. The response of the activated sludge process to acute and chronic toxicity is monitored by means of a batch short-term respirometer. Generic inhibition functions have been introduced to model the effect of a toxicant on heterotrophs and nitrifiers growth and death. Constant inhibition kinetic parameters are used for acute toxicity modelling. For chronic toxicity modelling the variability of toxicant concentration and characteristics is taken into account by a transformation of these kinetic parameters into state variables.

Keywords: benchmarking, fault detection, inhibition, respirometry.

1. INTRODUCTION

BSM1, BSM1_LT and BSM2 are benchmarking simulation tools which have been proposed to test and compare control strategies on wastewater treatment plants based on activated sludge (Jeppsson and Pons, 2004; Jeppsson et al., 2006). BSM1 is focused on the activated sludge bioreactor (with a two-compartment anoxic zone followed by a three-compartment aerobic zone) combined with a final clarifier. Its long-term version, BSM1_LT, has been set up to test monitoring and fault-detection systems. BSM2 includes BSM1 but deals also with the wastewater pre-treatment (in a primary settler) and sludge treatment (by thickening, anaerobic digestion and dewatering).

Managers of large-scale urban wastewater treatment plants are often concerned by the discharge in the sewage network of toxic substances which can be harmful for the bacteria involved in the biotreatment or/and which can deteriorate the quality of the sludge in agricultural use.

Copp and Spanjers (2004) have evaluated a toxicity mitigation control strategy on BSM1. However the toxicant was only affecting heterotrophic behaviour, when many reports in literature indicate that nitrifiers (autotrophs) are more sensitive than heterotrophs to toxic.

The aim of the present contribution is to provide a generalized framework for the implementation of toxic inhibition in the activated sludge process. Two types of inhibition are however discussed: acute inhibition resulting from a large pulse of a toxicant discharged in the sewers and chronic inhibition which results from the numerous toxic substances discharged at small doses in a large urban environment.

In both cases the toxicity is monitored by means of a batch short-term respirometer (Le Bonté et al., 2005a). Although oxygen uptake rates can be extracted from the physiological model (ASM1), a precise modelling of the respirometer has been preferred: design parameters such as the sludge/feed ratio, the time sequence, etc can be investigated.

2. BASIC INHIBITION MODELLING

Growth rate changes are generally modelled by comparison with the inhibition of enzyme-catalyzed reactions. The classical Michaelis-Menten mechanisms can be modified by adding two steps

describing the behaviour of an inhibitor (I). The general expression:
$r_X = \mu SX/(K_s + S)$ can be replaced by:

$$r_X = \frac{\mu SX}{(1+[I]/K_{I1})K_s + (1+[I]/K_{I2})S} \qquad (1)$$

Table 1 summarizes the relations between K_{I1}, K_{I2} and the different types of inhibition.

Table 1: Types of inhibition

Type of inhibition	$1+[I]/K_{I1}$	$1+[I]/K_{I2}$
None	1	1
Competitive	>1	1
Incompetitive	1	>1
Mixed	>1	>1

It can be seen from Eq.1 that the key parameter is the ratio $[I]/K_I$ which governs the extent of inhibition and not just [*I*] or K_I.

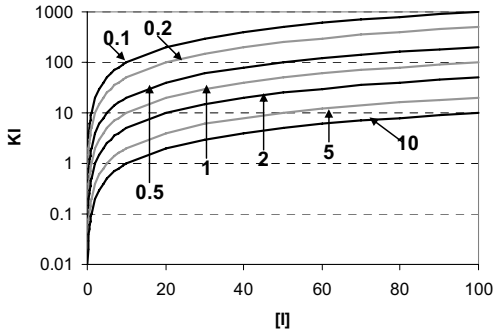


Fig. 1. Relationship between [*I*] and K_I for various values of $[I]/K_I$

A further effect of the toxicant could be an increase of the death rate. A similar approach is used: $r_d = -bX$ becomes:

$$r_d = -bX(1+[I]/K_{I1})^{\alpha}(1+[I]/K_{I2})^{\beta} \qquad (2)$$

α and β balance the effect of inhibition between the growth and the death rates. No toxic effect has been applied to the hydrolysis steps.

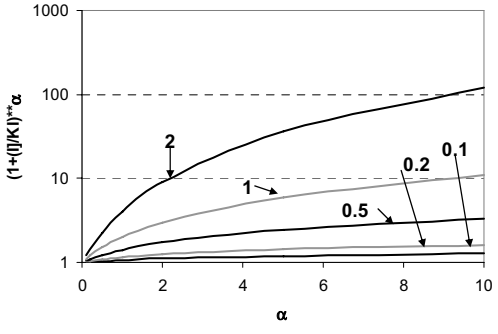


Fig. 2. Relationship between $(1+[I]/K_{I1})^{\alpha}$ and α for various values of $[I]/K_I$

Finally the toxicant can be degraded chemically or biologically or removed physically of the system (by stripping for example). This is modelled by a general removal rate:

$$r = -d \cdot [I]^{\gamma} \qquad (3)$$

2. ACUTE AND CHRONIC INHIBITION

Acute inhibition has been simulated by the direct addition of a soluble toxicant of given characteristics (K_{I1}, K_{I2}, α and β for heterotrophs and nitrifiers, *d* and γ) at the inlet of the biological reactor for BSM1 and BSM1_LT and of the primary settler for BSM2). The time of injection can be selected as well as the injection profile (Fig. 3.)

Chronic inhibition results from the presence in the wastewater of toxicants of variable nature and concentration. In order to take the toxicant variable nature into account, its characteristics have been transformed into state variables to which pseudo-mass balances can be applied. In Eq. 4 an example is given for K_{I1} for a biological reactor compartment *i* of volume V_i (Fig. 3):

$$dK_{I1}(i)/dt = (Q_i K_{I1}(i) - Q_{i-1}K_{I1}(i-1))/V_i \qquad (4)$$

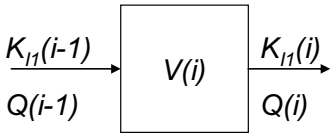


Fig. 3. Mass balance on a inhibition kinetic parameter

Similar equations have been built for the nine other parameters. There is no theoretical reason to apply such dynamics to the inhibition kinetic parameters. These variation laws are only seen as a mean to translate easily in a simulation environment the variation of the nature of the toxicants. The inhibition kinetic parameters have been added in the influent files available on the website correspondingly (http://www.benchmarkWWTP.org).

3. RESPIROMETER MODEL

The batch respirometer is operated sequentially with the following phases: filling, aerobic reaction, emptying-cleaning. Its operational parameters are: the wastewater sample /sludge volume ratio, the oxygen transfer rate, the temperature, the aerobic reaction time. The biological model used in the respirometer is the same as in the plant biological reactor. The sludge is supposed to be collected at the beginning of each cycle on the external recycle line (i.e. from the secondary clarifier underflow). The dissolved oxygen concentration in the respirometer is monitored by a probe with first-order response characteristics. The wastewater sample can be an instantaneous sample or an average sample collected over the previous respirometric cycle. This second filling strategy can be set up to correct the discrete mode of operation of the respirometer. The instantaneous oxygen rate in the respirometer (OUR_{resp}) is calculated from the dissolved oxygen data:

$$OUR_{resp} = K_l a_{resp} \cdot (C_S - C) - dC/dt \qquad (5)$$

where $K_l a_{resp}$ is the mass transfer coefficient in the respirometer, C the dissolved oxygen concentration measured by the probe, C_S the dissolved oxygen concentration at saturation at the respirometer temperature. The inhibition kinetic parameters are a linear combination of their values in the wastewater sample and in the sludge from the recycle line.
For each cycle, the total amount of oxygen consumed by the bacteria is calculated:

$$VO_2 = \int OUR_{resp} \cdot dt \qquad (6)$$

and the maximal OUR_{resp} observed during the cycle (OUR_{max}) is detected.

4. BENCHMARK IMPLEMENTATION

A FORTRAN implementation of BSM1/BSM2 has been used. The detailed equations can be found in Copp et al. (2002). The system has been operated in open-loop with a stabilization period of 50 days for constant inputs and a dynamic stabilization period of two weeks using the dry weather data file. For chronic toxicity tests, a four weeks dry weather data file has been built by repetition of the original dry weather data file. Inhibition kinetic parameters have been then added for chronic toxicity tests. The respirometer has a working volume of 2L and is operated at 20°C. The sludge and wastewater volumes are 1.6 and 0.4 liters, respectively. The oxygen mass transfer coefficient is 20 hr^{-1}. The cycle duration is 30 min, with 15 min for respiration monitoring for 15 min of cleaning.

4. RESULTS

4.1 Acute toxicity

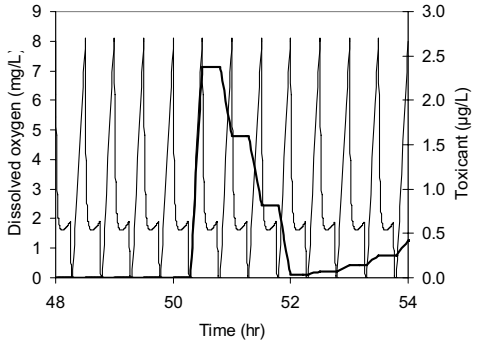
Table 2 summarizes the simulation conditions for the acute toxicity tests. Figure 4 presents the reference respirometer response in the case of the discharge in wastewater of a nonbiodegradable toxic substance. The increase in the toxicant concentration after 52 hrs is due to its gradual appearance in the sludge recycle line where the sludge feeding the respirometer is sampled.

Table 2: Acute inhibition tests conditions

Case	A	B	C	D
$K_{I1,het}$(µg/L)	10^4	1	0.1	1
$K_{I2,het}$(µg/L)	10^4	10^4	0.1	1
$K_{I1,nit}$(µg/L)	10^4	10^4	10^4	0.5
$K_{I2,nit}$(µg/L)	10^4	10^4	10^4	0.5
α_{het}	0.1	0.1	0.1	1
β_{het}	0.1	0.1	0.1	1
α_{nit}	0.1	0.1	0.1	1
β_{nit}	0.1	0.1	0.1	1
d (µg/L/hr)	0	0	0	0
γ	1	1	1	1

In Figure 5 the effect of a pulse of toxicant with a competitive inhibition effect on heterotrophs is shown. A 30% decrease of the OUR_{max} is observed but the oxygen volume consumed is only slightly affected.

(a)



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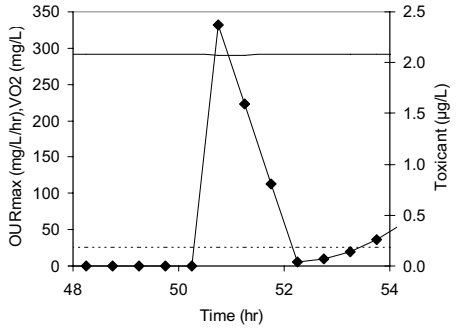
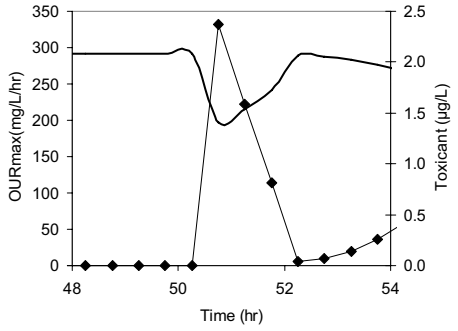


Fig. 4. Acute inhibition case A. (a) Dissolved oxygen versus time in the respirometer. (b) OUR_{max} and VO_2 in the respirometer.

(a)



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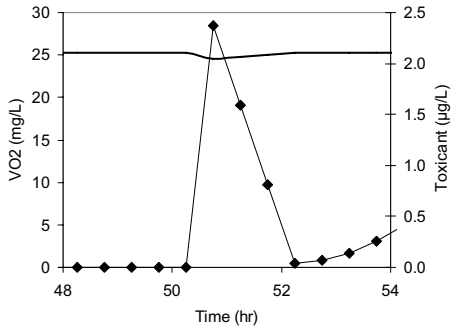
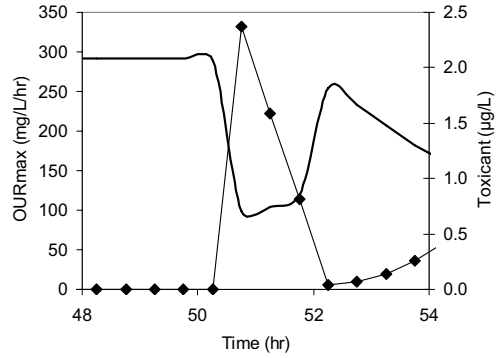


Fig. 5. Acute inhibition case B. (a) OUR_{max} versus time in the respirometer. and (b) VO_2 in the respirometer.

(a)



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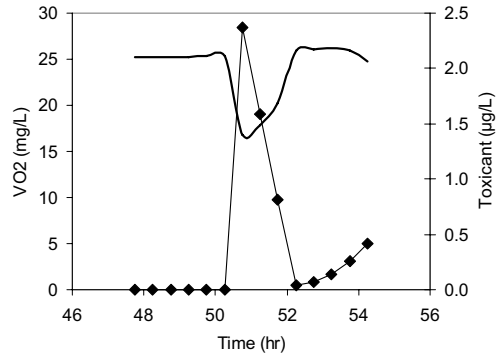
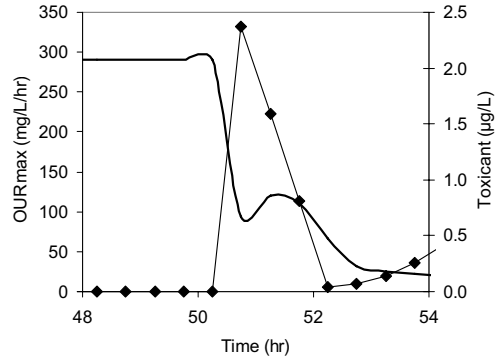


Fig. 6. Acute inhibition case C. (a) OUR_{max} versus time in the respirometer. and (b) VO_2 in the respirometer.

(a)



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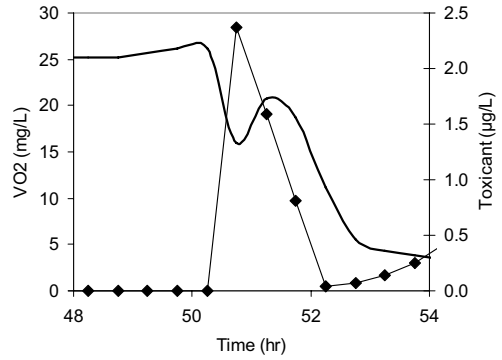


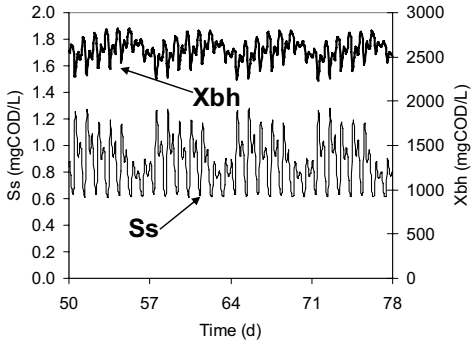
Fig. 7. Acute inhibition case D. (a) OUR_{max} versus time in the respirometer. and (b) VO_2 in the respirometer.

In Figure 6 (case C) both heterotrophs and autotrophs are inhibited although the toxicant does not increase the death rates of both types of bacteria. OUR_{max} and VO_2 decrease by a factor of 60% and 30% respectively. Finally Figure 7 depicts the worst case with an increase of the microbial death rate: ultimately the plant does not recover from that toxic event.

4.1 Chronic toxicity

Figure 8 describes the normal operation of BSM1 at dynamic steady state from the point of view of the fifth compartment of the biological reactor (biodegradable soluble pollution, Ss and heterotrophic bacteria (Xbh)), the discharged effluent (ammonia (Snh) and nitrate (Sno)) and the summarized information obtained from the respirometer (VO2 and OURmax) between days 50 and 78.

(a)



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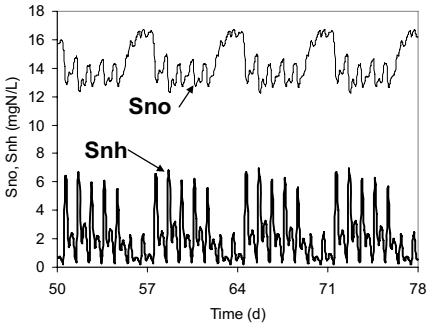


(c)

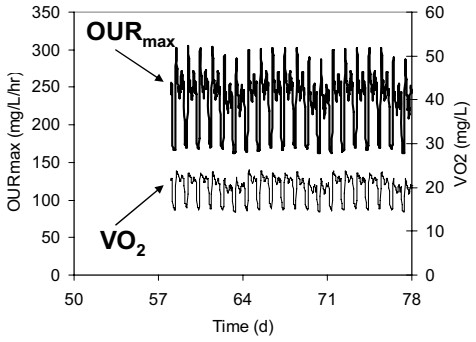


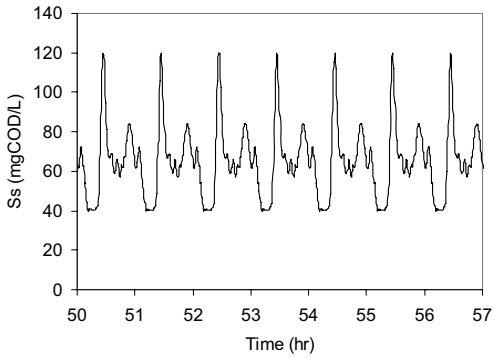
Fig. 8. Normal operation of BSM1, without inhibition. (a) Soluble biodegradable substrate (Ss) and heterotrophic biomass (Xbh) in the third aerated compartment; (c) Respirometric characteristics

Two chronic inhibition cases have been tested as described in Table 3. Figure 9 compares the variations of the biodegradable soluble substrate with those of the toxicant concentration in the plant influent for case E.

Table 3: Chronic inhibition tests conditions: averages and coefficient of variation (CV)

Case	E		F	
	Aver.	CV(%)	Aver.	CV(%)
Toxicant (µg/L)	2.53	57	0.25	57
$K_{I1,het}$(µg/L)	10	14.5	10	14.5
$K_{I2,het}$(µg/L)	10	14.5	10	14.5
$K_{I1,nit}$(µg/L)	5	14.5	5	14.5
$K_{I2,nit}$(µg/L)	5	14.5	5	14.5
α_{het}	1.12	6.4	1.12	6.4
β_{het}	1.12	6.4	1.12	6.4
α_{nit}	1.12	6.4	1.12	6.4
β_{nit}	1.12	6.4	1.12	6.4
d (µg/L/hr)	2.5	57	2.5	57
γ	1	0	1	0

(a)



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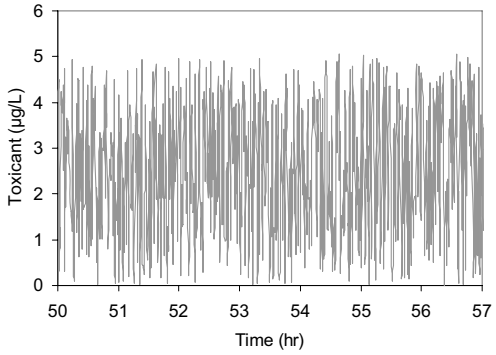
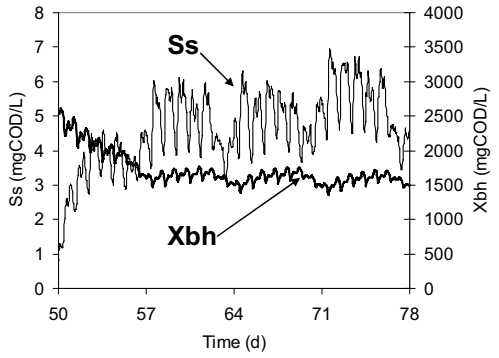


Fig. 9. Influent wastewater characteristics for test case E between day 50 and day 57 (a) Soluble biodegradable substrate (Ss); (c) Toxicant concentration

As shown in Figure 10, case E induces a severe breakdown of BSM1 with a 40% decrease of the average heterotrophic biomass concentration. Nitrification stops completely with the death of the nitrifiers. The ammonia concentration in the effluent is higher than in the influent as ammonification is not inhibited. The information provided by the respirometer fit these observations with a decrease of VO_2 and of the average OUR_{max}, which is divided by 3 with respect to the non inhibited case. In the BSM environment the global effluent quality is given by the E.Q. criterion, which is a linear combination of the effluents characteristics (BOD_5, COD, suspended solids, nitrogen substances). It is 1.3 times larger in case E than in the no inhibited situation. In the framework of testing monitoring and fault detection systems, it is obviously not a good idea to have a full breakdown of the plant. The range of variation of the inhibition kinetic parameters as well as of the toxicant concentration should be adjusted. In case F the toxicant concentration was decreased which gives a more reasonable behaviour of the plant as shown in Figure 11.

(a)



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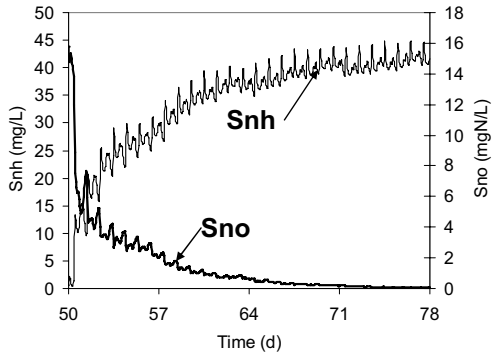

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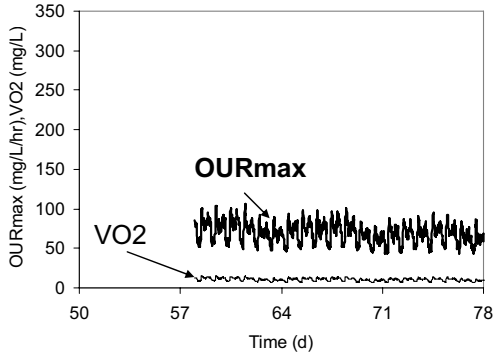
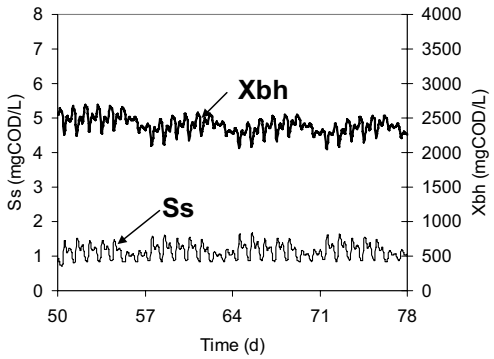


Fig. 10. Chronic inhibition (case E). (a) Soluble biodegradable substrate (Ss) and heterotrophic biomass (Xbh) in the third aerated compartment; (c) Respirometric characteristics.

(a)



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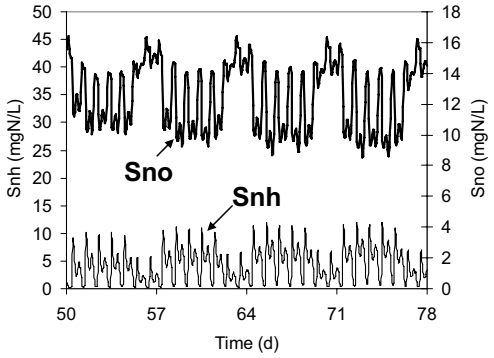

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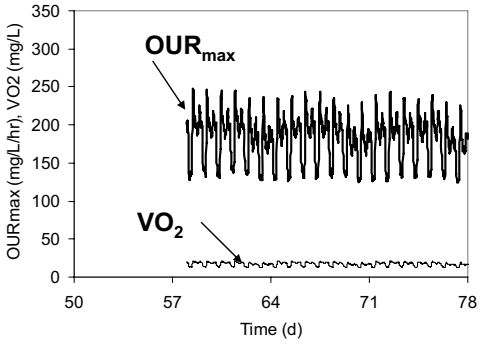

Fig. 11. Chronic inhibition (case F). (a) Soluble biodegradable substrate (Ss) and heterotrophic biomass (Xbh) in the third aerated compartment; (c) Respirometric characteristics.

5. CONCLUSIONS

The activated sludge process of wastewater treatment plant benchmark simulation models (BSM1, BSM1_LT and BSM2) have been modified to include the effect of soluble, biodegradable or non biodegradable toxic substances for acute and chronic inhibition configurations. Generic inhibition functions have been introduced to model the effect of a toxicant on heterotrophs and nitrifiers growth and death. Constant inhibition kinetic parameters are used for acute toxicity modelling. For chronic toxicity modelling the variability of toxicant concentration and characteristics is taken into account by a transformation of these kinetic parameters into state variables, to which mass balances have been applied. This allows keeping track of the changes in the toxicant characteristics over the system. By a proper choice of the range of variation of the model parameters, a realistic behaviour of the BSM1 plant is obtained, to which fault detection strategies could be applied (Le Bonté et al., 2005b)

On-going work is aimed at the case of insoluble toxicant or toxicant adsorbed on particulate pollution, that would be recycled through the whole BSM2 plant though the sludge treatment section.

DISCLAIMER

The content of the paper reflects the sole ideas of the author and is not endorsed by the IWA Task Group on Benchmarking of Control Strategies.

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