A calibration protocol of a one-dimensional moving bed bioreactor (MBBR) dynamic model for nitrogen removal

U. Barry, J.-M. Choubert, J.-P. Canler, A. Héduit, L. Robin and P. Lessard

ABSTRACT

This work suggests a procedure to correctly calibrate the parameters of a one-dimensional MBBR dynamic model in nitrification treatment. The study deals with the MBBR configuration with two reactors in series, one for carbon treatment and the other for nitrogen treatment. Because of the influence of the first reactor on the second one, the approach needs a specific calibration strategy. Firstly, a comparison between measured values and simulated ones obtained with default parameters has been carried out. Simulated values of filtered COD, NH_4-N and dissolved oxygen are underestimated and nitrates are overestimated compared with observed data. Thus, nitrifying rate and oxygen transfer into the biofilm are overvalued. Secondly, a sensitivity analysis was carried out for parameters and for COD fractionation. It revealed three classes of sensitive parameters: physical, diffusional and kinetic. Then a calibration protocol of the MBBR dynamic model was proposed. It was successfully tested on data recorded at a pilot-scale plant and a calibrated set of values was obtained for four parameters: the maximum biofilm thickness, the detachment rate, the maximum autotrophic growth rate and the oxygen transfer rate.

Key words | 1D-dynamic model, calibration procedure, MBBR, nitrogen removal, pilot-scale plant, sensitivity analysis

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INTRODUCTION

Over the last decades, the increasing interest in biofilm processes led to the development of the moving bed bioreactor process (MBBR). This process consists of the growth of biomass inside a biofilm attached to freely moving carriers. Air is supplied to meet the oxygen requirements of the biomass and to mix carriers. Reactors are equipped with sieves at their outlet. This process allows the retention of a significant biomass quantity attached to carriers, without recirculation contrary to the integrated fixed-film activated sludge process (IFAS). The MBBR can be used for the removal of carbonaceous compounds with one reactor (Ødegaard *et al.* 1999) and for nitrogen removal with two successive reactors (Andreottola *et al.* 2000).

In order to design and improve the knowledge about the various processes occurring in the MBBR, several dynamic models have been proposed. A zero-dimensional model has been proposed (Plattes *et al.* 2006). It is simple to use but is a diffusion-free model. One-dimensional models consider diffusion and an homogeneous repartition of the biofilm on the surface of carriers (parallel to substratum), assuming a negligible gradient parallel to the substratum (Eberl *et al.* 2006). Perpendicular to the substratum, the biofilm is divided into several layers that are considered as completely mixed reactors. Two and three-dimensional models integrate a heterogeneous distribution of particulate and dissolved compounds (Eberl *et al.* 2006). Nevertheless, they require the use of high skills and a powerful computer, and this limits a practical use by engineering contrary to zero- or one-dimensional models.

For biofilm models adapted to MBBR process, no specific calibration procedure has been proposed (Boltz *et al.* 2010) as it is the case for activated sludge (IWA Task Group on Good Modelling Practice, in press) or biofilter process (Vigne *et al.* 2007). Thus, a calibration procedure was found to be necessary to calibrate the MBBR model on recently developed carriers.

The aim of this work was to propose a calibration strategy to determine the parameters of a one-dimensional MBBR dynamic model in nitrification treatment, with recently developed carriers. Following a sensitivity analysis,

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the strategy was developed, and was applied to experimental data.

MATERIALS AND METHODS

The MBBR pilot-scale plant

A pilot-scale unit was fed by the municipal wastewater of Fontaines sur Saône (France, 30,000 PE) after pre-treatment (grit and grease removal, and no primary settling tank). It consisted of two aerobic reactors in series filled with carriers B2 and B3 (Figure 1) respectively. The first tank (Reactor C) had a 65% filling ratio developing a total theoretical surface area of 1,404 m^2. The second tank (Reactor N) had a 35% filling ratio developing a total theoretical surface area of 803 m^2 (Figure 1). During 63 days, the pilot was fed with a constant hourly flow rate, with 13.5 m^3/d for the first 48 days, and 27 m^3/d for the remaining 15 days. An air flow rate (medium bubbles) of 12–20 Nm^3/h was maintained in both reactors, the water temperature was in a range of 9–11 °C and pH between 7 and 8. The average applied surface loading rate was 1.5 g filtered COD/m^2 d on the reactor C (±0.8 g/m^2 d) and 0.6 g NH_4-N/m^2 d on the reactor N (±0.3 g/m^2 d).

On-line data recording was carried out for influent conductivity, temperature, oxygen, redox potential and pH. Twice a week, daily flow proportional samples were collected in the inlet/outlet of both reactors with an automatic refrigerated sampler. Chemical analysis of classical parameters (TSS, COD, NH_4-N, NO_2-N, NO_3-N, TKN) was carried out according to standard methods (APHA 2005). Batch experiments were regularly applied to samples of carriers to determine the biofilm thickness (L_f) and the maximum nitrification rate (noted NPR_{max} defined as $NPR_{max} = \mu_{A,max} * Xba/Y_A$) according to protocols published in Vigne *et al.* (2010) and Melcer *et al.* (2003).

Conceptual MBBR model (44 parameters)

The dynamic MBBR model chosen is the hybrid system included in GPS-X® 5.0 (Hydromantis Inc.). It combines a one-dimensional model of a suspended growth, based on the ASM1 (Henze *et al.* 1987) and a biofilm model (Spengel & Dzombak 1992). This model, represented in Figure 2, integrates the main physical and biological mechanisms that occur in the MBBR process.

The one-dimensional MBBR model is composed of:

- *Hydraulic and spatial model*: the geometrical representation of the MBBR process consists of a section (substratum) with a surface area equivalent to the total surface developed by the carriers. The biofilm system is divided into n parallel layers (six by default in GPS-X®; Hydromantis 2006): one limit liquid layer ($k = 1$) and $n - 1$ biofilm layers ($k = 2 - n$) considered as completely mixed reactors (Figure 2).
- *Biofilm and transport model (21 parameters)*: the model is based on the model of attachment/detachment proposed by Spengel & Dzombak (1992). Transport and transfer mechanisms occur perpendicularly to these layers and regulate the concentrations in each biofilm layer. Soluble compounds are transferred through the different layers by diffusion. Distribution of particular compounds inside the biofilm layers is calculated thanks to an internal solids exchange rate. Moreover, particular compounds attachment/detachment mechanisms occur at the biofilm surface.

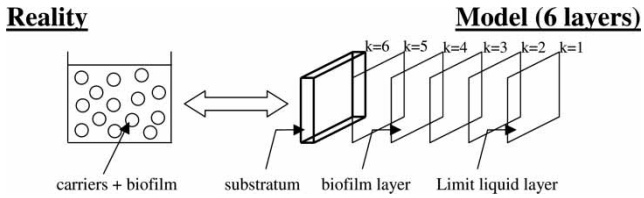

Figure 2 | Schematic representation of one-dimensional MBBR model (from Hydromantis 2006).

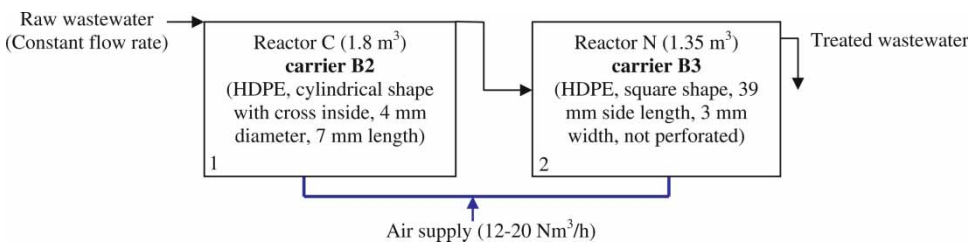

Figure 1 | Schematic representation of the pilot-scale plant.

- *Biological conversion of substrates (23 parameters)*: biological reactions are described with the MANTIS model (Hydromantis 2006) which is a modified ASM1 model (Henze *et al*. 1987) including two extra processes: (i) a growth dependency of the heterotrophic biomass with nitrates concentration, and (ii) nitrate utilization for these growths.

Simulations

A simulation of a 63 days period (from 4 January to 8 March 2010) was carried out with the MBBR model operated under COD limited regime. A first set of parameters values was used (set 1). It was obtained with default values and some of them were updated after a literature review for physical, diffusion and kinetics parameters (Horn & Morgenroth 2006; Boltz *et al*. 2009; Choubert *et al*. 2009). Another set of parameters was calibrated to improve the fit of simulated values with measured values (set 2).

The COD fractions of the wastewater were determined with COD values measured in raw wastewater, wastewater released by reactor C and rector N (daily average composite samples). For raw wastewater, COD fractions were changed and maintained constant at 11 instants as seen in Table 1.

To evaluate the accuracy of the model, the simulated results were compared with the daily average concentrations with relative mean deviation (RMD) and mean deviation (MD):

$$\mathrm{RMD} = 1/n * \sum(|C_{\mathrm{simulated}} - C_{\mathrm{measured}}|/C_{\mathrm{measured}}) \quad (1)$$

$$\mathrm{MD} = 1/n * \sum|C_{\mathrm{simulated}} - C_{\mathrm{measured}}| \quad (2)$$

where n is the number of experimental values, C the daily average concentration of substrate that is monitored at the outlet of a reactor; simulated and measured refer to simulated concentration and measured concentration respectively.

Sensitivity analysis

For each parameter, simulations were carried out with default parameter values modified by ±30% or ±50%, and the modifications of the output variables were monitored. This sensitivity analysis was carried out with a constant surface loading rate of 2.1 g BOD_5/m^2 d and the following influent characteristics (TSS = 225 mg/L, COD = 411 mg/L, filtered COD = 98 mg/L, BOD_5 = 212 mg/L, TKN = 56 mg/L, NH_4-N = 30 mg/L). Then, a sensitivity analysis was carried out to estimate the impact of the fractionation of COD and nitrogen of the raw influent on the output variables of the model. A modification by ±20% was applied on initial values of the fractions Ss (20% of 411 mg COD/L), Si (4% of COD), Xs (55% of COD), Xi (15% of COD), Snh (30 mg N/L), Snd and Xnd (10 mg N/L). Moreover, the effects of autotrophic mass entering into the reactor N were studied for two autotrophic concentrations of 0 and 1.65 mg COD/L. The concentrations were Si = 30 mg COD/L, Ss = 2.65 mg COD/L, Xi = 138 mg COD/L, Xs = 11 mg COD/L, Xbh = 71.5 mg COD/L, So = 3.2 mg O_2/L, Snh = 6.3 mg N/L, Snd = 1.2 mg N/L, Xnd = 0.2 mg N/L, Sno = 13.2 mg N/L.

RESULTS AND DISCUSSION

Sensitivity analysis

The sensitivity analysis leads to the proposal of a calibration protocol enabling correct modification of the parameters of the 1D-MBBR model. The most sensitive parameters for reactor N were gathered into three categories and presented in Table 2 for the variables in the effluent (TSS, filtered

Table 1 | Conditions of simulation (flow rate, surface loading rates on reactor C and N)

Simulation days	0	10	14	17	39	42	49	52	56	59	62
Flow rate (m^3/d)	13.7	13.7	13.7	13.7	13.7	13.7	27	27	27	27	27
Load on reactor C (g COD/m^2 d)	3.2	2.6	2.6	3	4.4	4	5.4	6	8	7	9.9
Load on reactor N (g NH_4-N/m^2 d)	0.4	0.1	0.3	0.3	0.7	0.5	0.7	0.9	1.1	1	1.3
Fractionation range (mg COD/L)	Ss: 9–46, Si: 30, Xs: 77–215, Xi: 68–162, Xbh: 5, Snh: 12–46 mg N/L, Snd = Xnd: 1–3 mg N/L, Sno: 0.5–2 mg N/L										

Table 2 | Sensitivity of selected output variables to the parameters of reactor N

			In treated effluent			In reactor N		
	Parameters of reactor N	**Unit**	**TSS**	**Filtered COD**	**NH_4-N, NO_x-N**	**$M_{biofilm}$**	**L_f**	**NPR_{max}**
Biological conversion	Maximum heterotrophic growth rate ($\mu_{H,max}$)	d^{-1}	−	+	−	−	−	−
	Maximum autotrophic growth rate ($\mu_{A,max}$)	d^{-1}	−	−	+	−	−	++
	Autotrophic decay rate (b_A)	d^{-1}	−	−	+	−	−	++
	Ammonification rate (k_A)	m^3/g COD d	−	−	+	−	−	−
	Ammonia half saturation coefficient (K_{na})	g N/m^3	−	−	++	−	−	−
Transport model	Attachment rate (r_{att})	m/d	−	−	−	++	++	−
	Detachment rate (k_{det})	kg/m^2 d	−	−	−	++	++	−
	Internal solids exchange (k_{exch})	m/d	−	−	−	−	−	+
Biofilm model	Maximum biofilm thickness ($L_{f,max}$)	m	−	−	+	++	++	−
	Dry material content of biofilm (DM)	−	−	−	−	++	−	++
	Mean density of wet biofilm (ρ_w)	kg/m^3	−	−	−	++	−	++

−: no influence (<5%), +: little influence (5 to 10%), ++ : strong influence (>10%).

COD, NH_4-N and NO_x-N) and in the reactor N ($M_{biofilm}$, L_f, NPR_{max}).

Considering the filtered COD concentration, the sensitivity analysis reveals that the maximum heterotrophic growth rate ($\mu_{H,max}$) has a little influence as confirmed by Boltz *et al.* (2010). The NH_4-N and NO_x-N concentrations in the reactor are affected by $\mu_{A,max}$, b_A, $L_{f,max}$ and k_A. We have obtained a strong influence of the attachment rate (r_{att}), the detachment rate (k_{det}) and the maximum biofilm thickness ($L_{f,max}$) on the biofilm thickness (L_f). These parameters influence the mass of biofilm ($M_{biofilm}$), but have no influence on the TSS released in the effluent. It could be explained by the fact that the value of the detachment rate coefficient (0.07 kg/m^2 d) provides simulated TSS lower than the observed values. Thus, a precise measurement of $M_{biofilm}$ and L_f in the reactor N will lead to a better estimation of the previously cited parameters. The maximum nitrate production rate (NPR_{max}) is strongly affected by the net autotrophic growth rate ($\mu_{A,max} - b_A$), the dry material content of biofilm (DM), the mean density of wet biofilm (ρ_w) and the internal solids exchange (k_{exch}). The measurement of NPR_{max} in a batch will estimate $\mu_{A,max}$ for a given value of b_A (0.13 d^{-1} at 10 °C).

The sensitivity analysis of the COD and nitrogen contained in the raw influent was studied (Table 3). A variation of Snh by 30% led to a strong variation of NH_4-N, NO_x-N and NPR_{max} (>10%) as was the case with Snd and Xnd. As a result, the Snh concentration in the inlet of reactor N should be monitored with on-line sensors. A variation of Ss by 20% leads to a NO_x-N variation higher than 10% but has no effect on filtered COD concentration in the effluent, nor on the mass and the thickness of biofilm. The filtered COD concentration in the effluent of reactor N is sensitive to Si.

Note that an incorrect estimation of the concentrations in the effluent of reactor C should have an effect on the output variables of reactor N, through the surface loading rate applied. The influence of the concentration of the

Table 3 | Sensitivity to the COD and nitrogen fractions in raw wastewater (reactor N)

				In treated effluent				In reactor N			
Fractions		**Default values**	**Variation (%)**	**TSS**	**Filtered COD**	**NH_4-N**	**NO_x-N**	**O_2**	**$M_{biofilm}$**	**L_f**	**NPR_{max}**
COD	Si	16 mg/L	40	−	++	+	−	−	−	−	−
	Xi	62 mg/L	35	+	−	+	−	−	−	−	−
	Ss	82 mg/L	20	−	−	+	++	−	−	−	+
	Xs	227 mg/L	20	++	−	++	++	−	+	+	++
Nitrogen	Snh	30 mg N/L	30	−	−	++	++	+	−	−	++
	Snd	10 mg N/L	50	−	−	++	+	−	−	−	+
	Xnd	10 mg N/L	50	−	−	++	+	−	−	−	+

− : no influence (<5%), + : little influence (5 to 10%), ++ : strong influence (>10%).

autotrophic biomass coming from reactor C has been studied with simulations. A concentration level of 1.65 mg COD/L caused an increase of NH_4-N of up 2 mg N/L (and a corresponding decrease of NO_x-N) in the effluent of reactor N. The influence is >10% for NPR_{max}.

Proposed calibration procedure and calibration of the model

The calibration procedure determined for the reactor N is shown in Figure 3.

The calibration procedure has been applied to the one-dimensional MBBR model for reactor N. Figure 4 represents, for set 1 (default parameters) and set 2 (calibrated parameters), the concentrations measured on daily average composite samples (spot samples) and the simulated values (continuous line) for the filtered COD, TSS, NH_4-N, NO_x-N and dissolved oxygen.

With default parameters values (set 1), the model does not fit the experimental concentrations for NH_4-N, NO_x-N and O_2. The simulated NH_4-N values are underestimated by 48% (SD: 7 mg/L), and NO_x-N overestimated by 110% (SD: 5 mg/L). These differences can be explained by an overestimation of the simulated nitrates production rate in reactor N (NPR_{max}), due to a bad estimation of the amount of autotrophic biomass, a too high autotrophic growth rate ($\mu_{A,max}$) or an efficient diffusion into the biofilm. Oxygen concentration is undervalued by 15% (SD: 2 mg O_2/L) certainly because of nitrifying activity. The simulated TSS values are overestimated by 43% compared with the measured values (SD: 50 mg/L). Thus, the detachment process in the model is overvalued. It is confirmed by the predicted mass of biofilm (3,249 g TSS) underestimated compared with measured value (4,853 g TSS). Finally, the simulated filtered COD is underestimated by 24% compared with the measured value (SD: 12 mg/L), particularly after the 39th day.

The time-course of the simulated output variables are reproduced with a better match with set 2. Four parameters were modified compared with set 1:

- $L_{f,max}$ was turned to 130 μm (150 μm in set 1). The values found in the literature were in the range 100–350 μm (Takács *et al.* 2007; Boltz *et al.* 2009).
- $k_{det} = 0.01$ kg/m^2 d (0.07 kg/m^2 d in set 1), $k_{attach} =$ 0.5 m/d. The values found in the literature were 0.0047 kg/m^2 d (Plattes *et al.* 2006) for carriers K_1 (500 m^2/m^3) and 0.001 kg/m^2 d for biofilter (Vigne *et al.* 2010). The higher values obtained may be due to higher detachment rate due to shocks between carriers.
- $\mu_{A,max}$ (20 °C) = 0.62 d^{-1} (1.4 d^{-1} in set 1) [assuming Arrhenius coefficient of 1.059 (Choubert *et al.* 2009)]. The values found in the literature were between 0.4 and 1.16 d^{-1} (Plattes *et al.* 2006; Mannina *et al.* 2007) for K_1 carriers (500 m^2/m^3).
- $k_{La} = 12$ h^{-1} (8 h^{-1} in set 1).

In order to evaluate the efficiency of the proposed calibration protocol, Table 4 presents the calculated mean

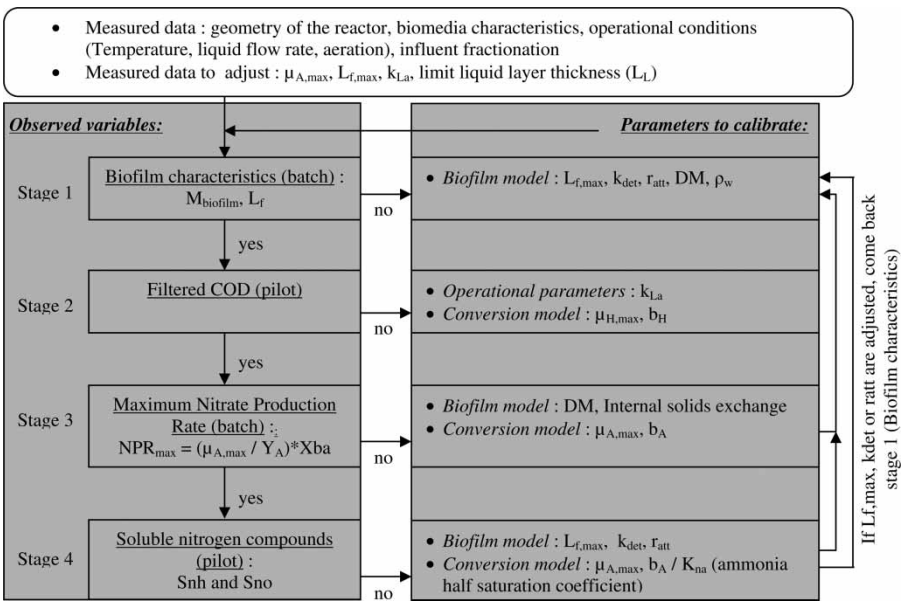

Figure 3 | Calibration procedure of MBBR 1D-model in reactor N.

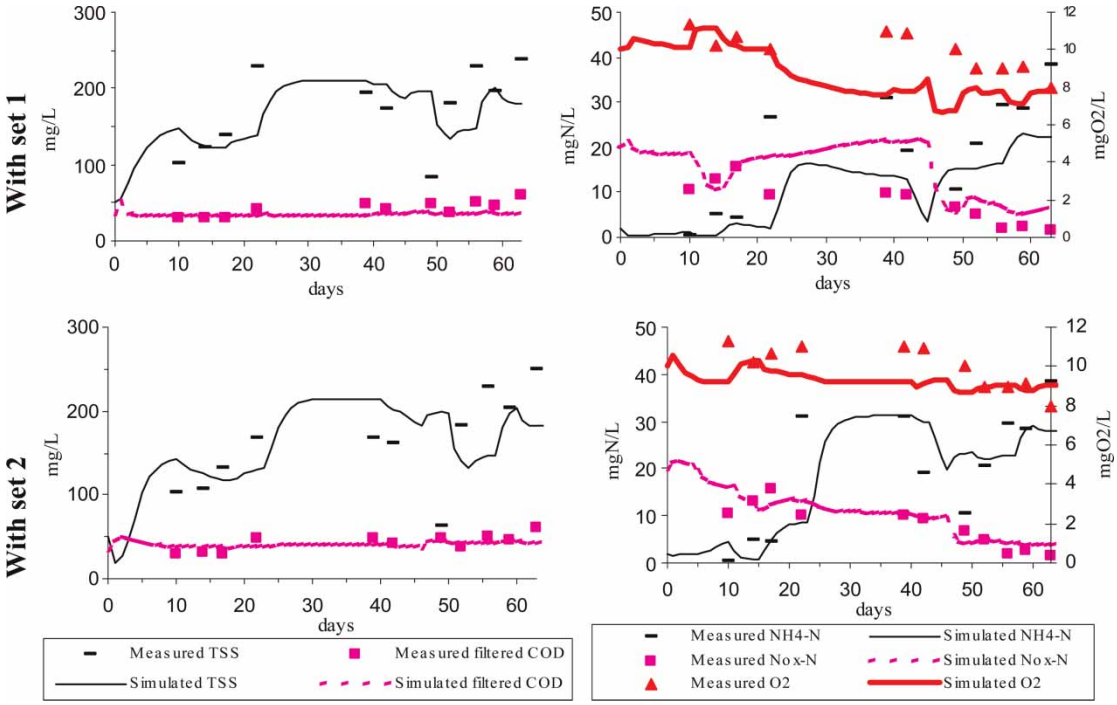

Figure 4 | Measured and simulated reactor N effluent concentrations with set 1 and set 2.

Table 4 | Relative mean deviation of measured and simulated values in reactor N obtained with default and calibrated parameters

	Default parameters (set 1)		Calibrated parameters (set 2)	
	RMD (%)	MD (mg/L)	RMD (%)	MD (mg/L)
TSS	43	50	41	48
Filtered COD	24	12	17	7
NH_4-N	48	7	45	7
NO_x-N	110	5	43	2
Dissolved oxygen	15	2	9	1

deviation (MD) and relative mean deviation (RMD) (Equations (1) and (2)) between simulated and measured data, with both default parameters (set 1) and calibrated ones (set 2). With calibrated parameters (set 2), we observed that the RMD of the concentrations in NO_x-N, O_2 and filtered COD decreased respectively from 110 to 43% (MD from 5 to 2 mg N/L), from 15 to 9% (MD from 2 to 1 mg O_2/L) and from 24 to 17% (MD from 12 to 7 mg COD/L). For the other variables, like TSS and NH_4-N, the fit has been slightly improved with mean deviations of 48 mg TSS/L and 7 mg NH_4-N/L respectively. Simulated masses were 8,133 and 5,134 g in reactor C and N, that match with measured masses of 8,926 g and 4,853 g in reactor C and N respectively once calibration was completed (set 2).

Even if the biofilm, the kinetic and the oxygen transfer parameters were modified, it is necessary to collect data to improve the match between simulated and measured concentrations. Two additional measurements should be carried out: the maximum autotrophic growth rate ($\mu_{A,max}$) with batch test protocol, and a systematic determination of COD fractions (e.g. Roeleveld & Van Loosdrecht 2002). Future sampling campaigns will be carried out every day during two weeks with an on-line measurement of NH_4-N in the inlet/outlet and NO_x-N in the outlet of reactor N. Thus, the rigorous application of the calibration protocol will provide a better match between simulated and measured data.

CONCLUSION

This work proposed a methodology to calibrate the biofilm model in GPS-X™. A comparison between measured and simulated data obtained with default model parameters allows the weaknesses of the 1D-model of MBBR to be highlighted. A sensitivity analysis then enabled classification of parameters between strong, little and no influence on output variables. Finally, a dynamic calibration protocol was proposed. The application of this protocol with experimental data allowed a good agreement between simulated

and measured values. A future on-line measurement campaign will lead to adjustment of the parameters set obtained.

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