Calibrating a side-stream membrane bioreactor using Activated Sludge Model No. 1

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Abstract Membrane bioreactors (MBRs) are attracting global interest but the mathematical modeling of the biological performance of MBRs remains very limited. This study focuses on the modeling of a side-stream MBR system using the Activated Sludge Model No. 1 (ASM1), and compares the results with the modeling of traditional activated sludge processes. ASM1 parameters relevant for the long-term biological behaviour in MBR systems were calibrated (i.e. $Y_H = 0.72$ gCOD/gCOD, $Y_A = 0.25$ gCOD/gN, $b_H = 0.25\,d^{-1}$, $b_A = 0.080\,d^{-1}$ and $f_P = 0.06$), and generally agreed with the parameters in traditional activated sludge processes, with the exception that a higher autotrophic biomass decay rate was observed in the MBR. Influent wastewater characterization was proven to be a critical step in model calibration, and special care should be taken in characterizing the inert particulate COD (X_I) concentration in the MBR influent. It appeared that the chemical–biological method was superior to the physical–chemical method. A sensitivity analysis for steady-state operation and DO dynamics suggested that the biological performance of the MBR system (the sludge concentration, effluent quality and the DO dynamics) are very sensitive to the parameters (i.e. Y_H, Y_A, b_H, b_A μ_{maxH} and μ_{maxA}), and influent wastewater components (X_I, S_s, X_s and S_{NH}).
Keywords Membrane bioreactor; modelling; parameter estimation; sensitivity analysis

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Introduction

Membrane bioreactor (MBR) systems are one of the most promising biological wastewater treatment techniques. Many studies have been performed on the modeling of MBR fouling problems, but the modeling of the biological performance of MBRs is still limited. The biological performance of a MBR and its description by the Activated Sludge model No.1 (ASM1) model might lead to characteristics that deviate significantly from the traditional activated sludge characteristics, due to the fact that: 1) membranes (microfiltration or ultrafiltration (UF)) serve as a barrier that completely retains biomass, reducing the wash-out of non-flocculating biomass (and thus reduces the selection of biomass species); 2) the biomass is imposed to high shear rate conditions in MBRs (especially in the side-stream configuration).

In this study, a lab-scale, side-stream MBR system is modelled using the ASM1, and the attention is focused on the comparison of the model characteristics of the MBR system with traditional activated sludge processes. Firstly, a steady-state MBR calibration was performed and the most sensitive parameters responsible for long-term behaviours were calibrated, i.e. the decay coefficients (b_H and b_A), the yield coefficients (Y_H and Y_A) and the inert particulate fraction of biomass (f_P) (Nowak *et al.*, 1999; Henze *et al.*, 2000; Vanrolleghem *et al.*, 2003). Meanwhile, the influent wastewater was completely characterized using two methods (physical–chemical and chemical–biological) for comparison purposes. A sensitivity analysis of all ASM1 parameters was performed afterwards to confirm that the calibrated parameters (b_H, b_A, Y_H, Y_A and f_P) are indeed the most sensitive parameters for steady-state behaviours. And finally, simulations of the DO concentration

dynamics and the corresponding sensitivity analysis (related to the short-term dynamic behaviour) were performed to verify the steady-state model calibration.

Methods

An aerobic side-stream MBR system was set up at the Van Hall Institute, the Netherlands. The schematic overview of the process layout is given in Figure 1. Pre-screened (1 mm micro screen) domestic wastewater of the Van Hall Institute was filled in a continuously stirred equalization tank (600 l) and afterwards pumped into a 300 l bioreactor (active volume 70–100 l), where it was mixed with the return sludge. Air was supplied from the bottom of the bioreactor through a diffuser (DO range 3–8 mg/l) and organic matter biodegradation and nitrification took place. A level controller was installed to control the filling volume of the bioreactor and the system was equipped with an external cooler to control the temperature between 22–28 °C. An online oxygen meter was installed in the bioreactor to monitor the DO concentration. The MLSS concentration of the bioreactor was controlled between 8–12 g/l, while the hydraulic retention time and sludge age were 8 hours and 20 days respectively.

The activated sludge in the bioreactor was pumped to a UF membrane (X-flow, F 5385) for biomass separation at constant pressure (0.5 bar) filtration conditions. The membrane material is PVDF, with 7 membrane tubes packed in one module. The diameter of the membrane tube is 8 mm and the length is 1 m. Air was introduced to the UF membrane co-currently with the sludge at a 2:1 ratio (the combined crossflow velocity was 4 m/s) to slough the membrane surface and reduce membrane fouling. The permeate (effluent) was collected outside the tube and the concentrated sludge was returned to the bioreactor. In order to keep a fixed HRT, the active volume of the MBR was adjusted daily due to the fact that the membrane fouling led to a decrease in permeate flux.

A simple static liquid and static air respirometer using a DO probe (LSS, Spanjers *et al.*, 1998) was built and the generated OUR profiles were used to characterize the influent wastewater and determine stoichiometric and kinetic parameters of ASM1. All respirometrical tests were carried out at T = 23 °C (identical temperature as the bioreactor). All the analyses were performed according to the *Standard Methods* (APHA, 1998). WEST (Hemmis NV, Kortrijk, Belgium) was applied as a tool for simulation and sensitivity analysis and the standard ASM1 (Henze *et al.*, 2000) was applied to model the biological behaviour of the MBR.

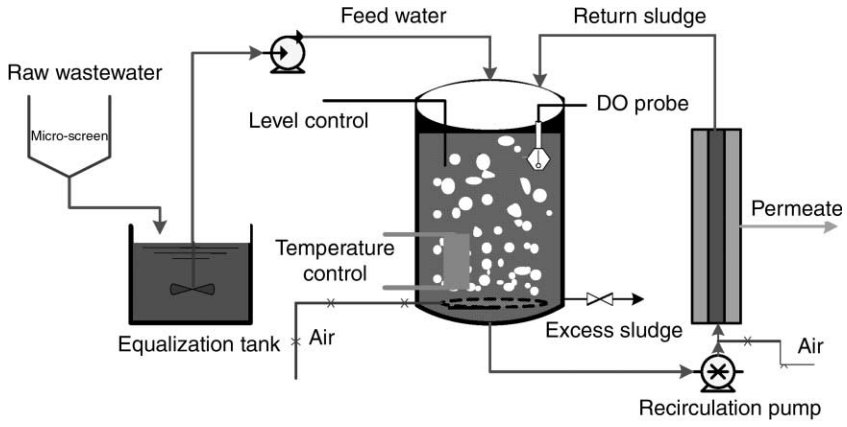

Figure 1 Scheme of a side-stream MBR system

Results and discussion

Steady-state calibration of stoichiometric and kinetic parameters

In this study, parameters responsible for the long-term behaviour of an activated sludge process were calibrated, i.e. the decay rate (b_H and b_A), the yield (Y_H and Y_A) and the inert particulate fraction of the biomass (f_P) (Nowak *et al.*, 1999; Henze *et al.*, 2000), while for the other parameters, default ASM1 parameters were applied (Henze *et al.*, 2000).

Decay rate (b'_H and b_A). The decay rate of the heterotrophic and autotrophic biomass was determined by: 1) taking a certain amount of activated sludge (7 kg) from the bioreactor and placing it into a non-fed aerated vessel for two weeks; and 2) taking a fixed amount of sludge (300 ml) each time (1–5 days) from the above vessel and transferring it into the respirometer to measure the exogenous respiration rate (r_{ex}) using excess acetic acid and ammonium chloride as substrate (Spanjers and Vanrolleghem, 1995). By plotting the exogenous respiration rate vs. time (Figure 2), the decay rate b'_H and b_A can be estimated by exponential curve fitting as $0.081\,d^{-1}$ and $0.080\,d^{-1}$. However, the estimated b'_H presented in Figure 2 is based on the 'traditional decay' concept and it must be translated to the 'death-regeneration' concept adopted in ASM1 (Henze *et al.*, 2000). Finally, the decay rates for ASM1 are $b_H = 0.25\ day^{-1}$ and $b_A = 0.080\ day^{-1}$ at T = 23 °C.

The b_H value of $0.25\,d^{-1}$ was lower than the default value in ASM1 ($0.4\,d^{-1}$ at 20 °C), which might be attributed to the absence of protozoa in the side-stream MBR, which probably reduced the predation and resulted in a lower decay rate (van Loosdrecht and Henze, 1999). The b_A in this MBR is significantly higher than the default values in ASM1 ($0.01\,d^{-1}$ at 20 °C), and it will result in a reduced nitrifier population and nitrification difficulties. The observed high b_A is probably due to the high turbulence existing in the UF module (4 m/s crossflow velocity imposed in 8 mm membrane tubes), since nitrifiers are generally regarded to be more sensitive to critical environmental conditions

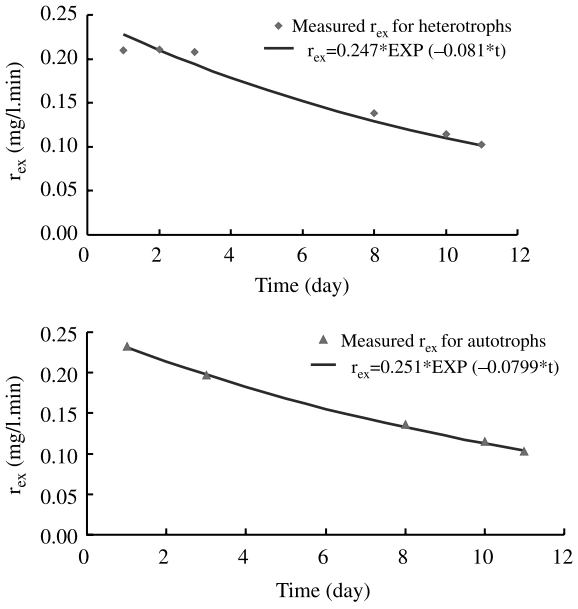

Figure 2 Determination of decay rate using respirometry (top b'_H; bottom b_A)

(van Loosdrecht and Henze 1999; Liebig *et al.*, 2001). However, further research is needed to investigate this interesting and remarkable difference.

Yield (Y_H and Y_A). 20.97 mg HAc (in COD unit) and nitrification inhibitor (ATU) were injected into the respirometric chamber at a S_0/X_0 ratio of 1/200. The OUR curve was obtained from the recorded DO profile in Figure 3 (left) and Y_H was estimated from the integral of the exogenous oxygen uptake rate (Vanrolleghem *et al.*, 1999). Oxygen was rapidly consumed by the heterotrophic biomass immediately after injection of the substrate (at 4 minutes) until substrate was depleted (28 minutes) and the endogenous respiration rate r_{en} was restored. From six duplicates, the Y_H value was estimated as 0.72 ± 0.05 gCOD/gCOD (average $\pm$ standard deviation). Using a similar method (but using NH_4Cl as substrate and no ATU addition), Y_A was estimated as 0.25 ± 0.01gCOD/gN.

The obtained Y_H (0.72 gCOD/gCOD at 23 °C) is a little bit higher than the default value in ASM1 (0.67 gCOD/gCOD at T = 20 °C), but it is probably due to the storage phenomenon (Majone *et al.*, 1999; van Loosdrecht and Heijnen, 2002). The obtained Y_A (0.25 gCOD/gN at 23 °C) is however, well in agreement with the default value in ASM1 (0.24 gCOD/gN at T = 20 °C).

Inert particulate fraction of the biomass (f_P). A fraction (typically 20%) of biomass is converted into inert particulate products during biomass decay (Henze *et al.*, 2000). This inert biological fraction is referred to as f'_p in the 'traditional decay' concept and the f_P defined in 'death regeneration' concept can be calculated using equation (1) (Henze *et al.*, 2000). As a result, f_P was estimated as 0.06.

$$f_P = \frac{f'_P(1 - Y_H)}{(1 - Y_H f'_P)} \tag{1}$$

where $Y_H = 0.72$ gCOD/gCOD and $f'_p = 0.2$ (Henze *et al.*, 2000).

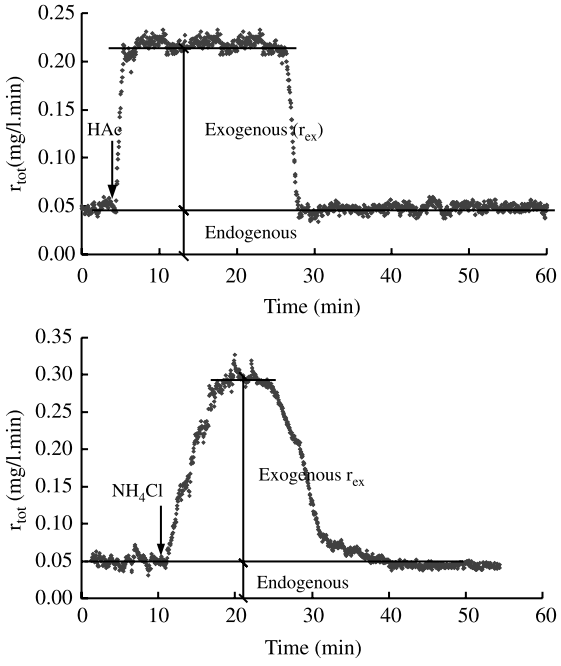

Figure 3 Determination of yield using respirometry (top Y_H; bottom Y_A)

Wastewater characterization using chemical–biological method

The "chemical–biological" methods mainly used OUR profiles to fractionate readily biodegradable (S_S) and slowly biodegradable COD (X_S). The soluble and particulate COD fraction of the influent wastewater (taken from the equalization tank) were determined by a 0.45 μm filter. After the analysis of 6 composite samples, the average soluble COD was 261 (± 84 mg/l) mg/l and the particulate COD was 318 (± 37) mg/l.

Readily biodegradable COD S_S. Raw wastewater was fed into a respirometer with an initial S_0/X_0 ratio of 1/200 and the nitrification was inhibited by ATU. A typical OUR_{ex} profile is shown in Figure 4. Oxygen consumption due to the degradation of S_S was identified as a peak, while the oxygen consumption due to the degradation of X_S was moderate and had a long tail due to the nature of the slow hydrolysis process (Vanrolleghem *et al.*, 1999). A straight line was fitted to the last part of the tail (40–140 minutes) to differentiate S_S and X_S. Consequently, S_S could be calculated from the area between the exogenous respiration curve and the extended fitting line (between 7–40 minutes), and the X_S could be calculated from the area under the line. From 16 OUR_{ex} curves, the S_S and X_S were estimated as 214 (± 52) mg/l and 253 (± 78) mg/l respectively.

Soluble inert COD S_I. The S_I fraction was assumed to be 90% of the effluent COD as suggested by Vanrolleghem *et al.* (2003). Thus, S_I was estimated as 33 (± 7) mg/l. The measured soluble COD by filtration was 261 mg/l, which was larger than the sum of S_S and S_I (214 + 33 = 247 mg/l). As suggested by Vanrolleghem *et al.* (2003), the remaining COD (S_{rest}, 14 mg/l) was calculated from equation (2) and it was afterwards added to the X_S.

$$S_{rest} = COD_{sol,inf} - S_I - S_S \quad (2)$$

Slowly biodegaradable COD X_S and inert particulate COD X_I. One method to estimate X_S is using the OUR profile (simultaneously determined with S_S in Figure 4). The result of this measurement was 253 mg/l. Another method to estimate X_S and X_I is the *trial and error* method, in which the measured and simulated sludge concentrations combined with COD mass balance (equation (3)) were compared to minimize the error (Vanrolleghem *et al.*, 1999; Henze *et al.*, 2000; Vanrolleghem *et al.*, 2003). As a result, X_I was obtained as 58 mg/l and X_S was 260 mg/l.

$$X_S = COD_{tot} - COD_{sol} - X_I \quad (3)$$

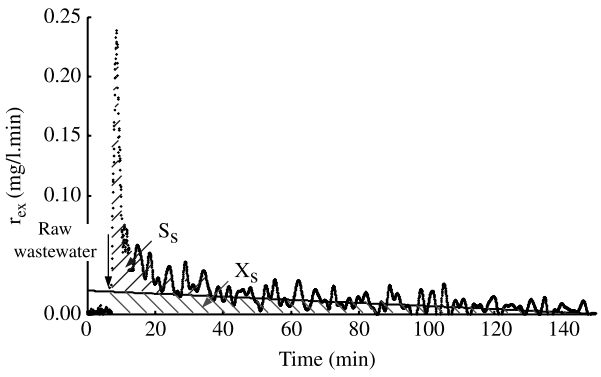

Figure 4 A OUR_{ex} profile to determine S_S and X_S

The X_S value obtained using these two independent methods have good agreements (253 mg/l using the OUR profile and 260 mg/l based on fitting the MLSS concentration). To minimize the error in the prediction of the MLSS concentration, the X_S value of 260 mg/l was adopted for all future work.

The characterization of nitrogen components used standard methods (APHA, 1998; Henze *et al.*, 2000). The wastewater characterization results (COD and nitrogen components) are summarized in Table 1.

Wastewater characterization using physical-chemical method

The "physical–chemical" methods mainly used filtration to fractionate them (Hulsbeek *et al.*, 2002), the details of which are not presented here and the results are summarized in Table 1.

Comparison of the methods of wastewater characterization and steady-state simulations

The results of the wastewater characterization using the chemical–biological and physical–chemical methods are summarized in Table 1. The steady–state simulation results using the calibrated stoichiometric and kinetic parameters and wastewater characterized by the two methods are presented in Figure 5. The largest difference between the two wastewater characterization methods occurred for the X_I value (58 mg/l and 141 mg/l) (Table 1), which resulted in a significant deviation of the simulated X_I concentration in the bioreactor (3230 mg/l using the chemical–biological and 8100 mg/l using the physical–chemical method respectively) (Figure 5 left). In terms of the total MLSS concentration in the bioreactor, the simulation results using the chemical–biological method showed a good agreement with the measured values due to the "trial and error" method, which minimized the deviation. However, the X_S value obtained from the OUR profile had only 7 mg/l deviation from the "trial and error" results as stated above. On the other hand, the physical–chemical method resulted in a significant deviation of the MLSS concentration when comparing the simulated (13245 mg/l) and measured (10020 mg/l) values. It should be noted that MBRs normally run at a condition of long sludge age and short hydraulic retention time, which results in the amplification of the X_I concentration in the bioreactor by the factor SRT/HRT (Grady *et al.*, 1999). As a result, it is crucially important to characterize X_I accurately and the chemical–biological method is therefore probably more suitable for MBR influent characterization.

In terms of effluent quality, both approaches showed good agreement with the measured values, suggesting that effluent quality is not very sensitive to the method of wastewater characterization and a good fit between the simulated and measured effluent quality cannot guarantee a successful influent characterization.

Table 1 Comparison of the results of wastewater characterization using the chemical–biological method and physical–chemical method

		Chemical–biological method	Physical–chemical method
COD_{tot} (579 mg/l)	S_I (mg/l)	33	33
	S_S (mg/l)	214	228
	X_I (mg/l)	58	141
	X_S mg/l)	260	177
TKN_{tot} (58 mgN/l)	S_{NH} (mgN/l)	48	
	S_{NI} (mgN/l)	0.6	
	S_{ND} (mgN/l)	4.1	
	X_{NI} (mgN/l)	0.6	
	X_{ND} (mgN/l)	4.7	

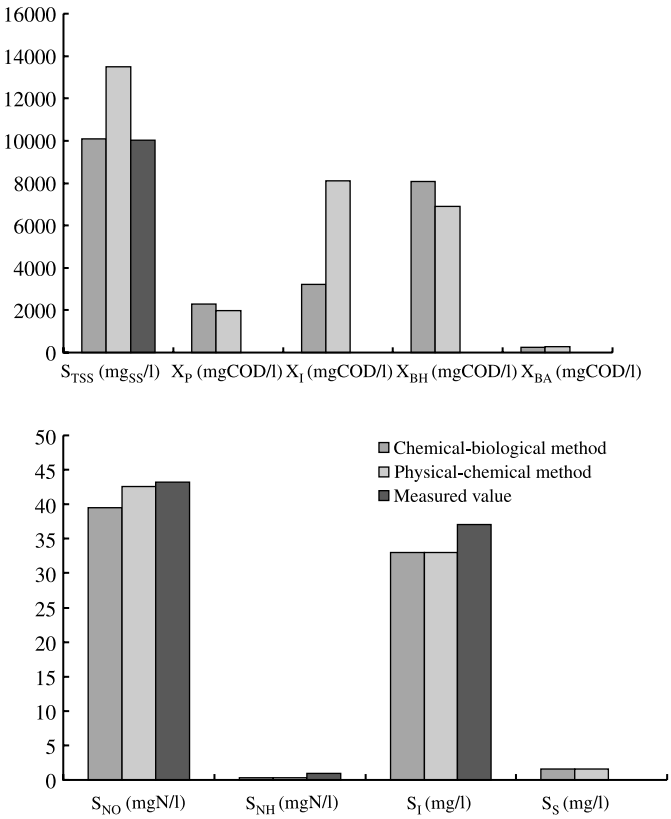

Figure 5 Comparison of simulated (using two wastewater characterization methods) and measured values in terms of sludge composition (top) and effluent quality (bottom) (the S_I in the effluent could not be measured directly, and the "measured" S_I value shown in the graph is actually the total COD of the MBR permeate)

Steady–state sensitivity analysis

In order to investigate whether the parameters that were calibrated during the steady-state model calibration (Y_H, Y_A, b_H, b_A and f_P) and the influent wastewater characterization (S_S, S_I, X_S X_I and S_{NH}, etc.) were indeed influencing the model output, (e.g. the simulated X_{TSS}, S_S, S_{NH} and S_{NO}), a steady-state sensitivity analysis was performed and the relative sensitivity function (RSF) was adopted to evaluate the sensitivity (Petersen, 2000). The results are summarized in Table 2.

Table 2 Steady-state sensitivity evaluation results

RSF	X_{TSS}	S_S	S_{NO}	S_{NH}
RSF $<$ 0.25 (not influential)	f_P, b_A, k_a, k_h, K_{NH}, K_{NO},K_{OA}, K_{OH}, K_S, K_X, μ_{maxA}, μ_{maxH},Y_A, S_{NO}	f_P, b_A, k_a, k_h, K_{NH}, K_{NO}, K_{OA}, K_{OH}, K_X, μ_{maxA}, Y_A, Y_H, S_S, S_{NH}, S_{NO}	f_P, b_A, k_a, k_h, K_{NH}, K_{NO}, K_{OA}, K_{OH}, K_S, K_X, μ_{maxA}, μ_{maxH}, Y_A, S_{NO}	f_P,,b_H, k_a, k_h, K_{NO}, K_{OA}, K_{OH}, K_S, K_X, μ_{maxH}, Y_A, Y_H, S_{NO}
0.25 $<$ RSF $<$ 1 (moderately influential)	b_H	b_H, K_S	b_H,Y_H	b_A, K_{NH}, S_{NH}
1 $<$ RSF $<$ 2 (very influential)	Y_H, S_{NH}	μ_{maxH}	–	μ_{maxA}, S_S
RSF $>$ 2 (extremely influential)	X_I, X_S, S_S	X_S	X_S, S_S, S_{NH}	X_S

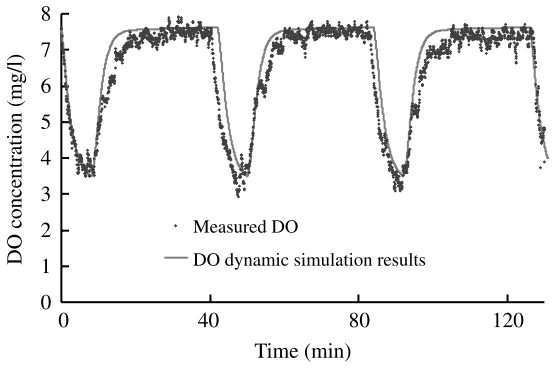

Figure 6 DO dynamic simulation

The influent wastewater characterization was *extremely* to *very* influential on the MLSS concentration and effluent quality, especially X_I, X_S, S_S and S_{NH}. Stoichiometric parameter (Y_H) and kinetic parameters (b_H, b_A, μ_{maxH} and μ_{maxA}) were *very* to *moderately* influential on the MLSS concentration and effluent quality. All *extremely, very and moderately* influential parameters (except for μ_{maxH} and μ_{maxA}) and wastewater components had been calibrated in this MBR system.

It appears (according to steady-state simulation and sensitivity analysis) that the calibration of the MBR was successful. However, since the steady-state simulation at one particular condition cannot guarantee the success of a MBR calibration, dynamic simulation is studied next.

Dynamic simulation of DO concentration

The influent flowing into the bioreactor was cyclic (approximately 8 minutes ON and 34 minutes OFF) controlled by a level control device. Consequently, the DO concentration in the bioreactor also showed a cyclic behaviour. The dynamics of DO concentration were simulated using the calibrated MBR model. The state variables of the steady-state simulation were used as initial conditions, and the characterized cyclic influent wastewater was used as input file in the dynamic simulation. The simulation results are compared with the online measured DO in Figure 6. A good agreement existed between the simulation results (solid line) and the DO real time results (the dots), which suggested and verified that the MBR model calibration was probably successful.

A sensitivity analysis was again performed for the DO concentration and results are presented in Table 3. The Influent wastewater components (S_S, S_{NH} and X_S) were *extremely* to *very* influential on the DO dynamics in the bioreactor. In addition to the calibrated parameters (Y_H and Y_A) and the estimated K_La (K_La was estimated by separate batch aeration tests), the DO concentration was also sensitive to μ_{maxA} and K_{NH}, which had not been calibrated. In order to get a better fit, μ_{maxA} and K_{NH} were slightly tuned, but no significant improvement could be found.

Table 3 DO sensitivity analysis under dynamic conditions

RSF	S_O
RSF $<$ 0.25 (not influential)	b_H, b_A, k_a, k_h, K_{OA}, K_{OH},K_{NO}, K_S, K_X, μ_{maxH}
0.25 $<$ RSF $<$ 1 (moderately influential)	μ_{maxA}, Y_H, K_{NH}, K_La, Y_A
1 $<$ RSF $<$ 2 (very influential)	X_S
RSF $>$ 2 (extremely influential)	S_S, S_{NH}

Conclusions

ASM1 parameters responsible for long-term biological behaviour in a side-stream MBR were calibrated, i.e. b_H, b_A, Y_H, Y_A and f_P. These parameters generally agreed with the parameter values found in traditional activated sludge processes, with the exception of the nitrifier decay rate. A significantly higher nitrifier decay rate ($0.080\,d^{-1}$) was observed in the side-stream MBR system, which was probably due to the higher shear stress in MBR systems.

Influent wastewater characterization was found to be a critical step in MBR model calibration. A chemical–biological method (mainly using respirometry) appeared superior to the physical–chemical method. Special care should be taken in determining X_I in a MBR influent characterization due to the characteristics of long SRT and short HRT in MBR systems. Sensitivity analyses for steady-state operation and DO dynamics suggested that the biological performance of the MBR system (the sludge concentration, effluent quality and the DO dynamics) is very sensitive to Y_H, Y_A, b_H, b_A, μ_{maxH} and μ_{maxA} and influent wastewater components (X_I, S_s, X_s and S_{NH}).

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