Evolution of an ASM2d-like model structure due to operational changes of an SBR process

G. Sin* and P.A. Vanrolleghem*,**

*BIOMATH, Ghent University, Coupure Links 653, B-9000 Gent, Belgium

**model*EAU*, Dépt. Génie Civil, Pavillon Pouliot, Université Laval, Québec G1K 7P4, Canada
(E-mail: *gurkan@biomath.ugent.be*; *peter.vanrolleghem@modelEAU.org*)

Abstract To model biological nitrogen and phosphorus removal systems with an affordable complexity, the ASM2d model structure is based on many assumptions. In this study, some of these assumptions, however, were observed to become invalid when the biological behaviour in the system altered in response to changes in the operation of the system, a pilot-scale N and P removing SBR. Particularly, the three applied operational scenarios resulted in three distinctive responses in the SBR, namely pronounced limitation of the hydrolysis of the organic nitrogen, nitrite build-up during aerobic conditions and also nitrite build-up during anoxic conditions. This shows that even for the same system with the same influent wastewater composition, the model structure of the ASM2d does not remain constant but adapts parallel to dynamic changes in the activated sludge community. On the other hand, the three calibrated ASM2d models still lacked the ability to *entirely* describe the observed dynamics particularly those dealing with the phosphorus dynamics and hydrolysis. Understanding the underlying reasons of this discrepancy is a challenging task, which is expected to improve the modelling of bio-P removing activated sludge systems.
Keywords Activated sludge; ASM2d; evolution; model structure; nutrient removal; SBR

Water Science & Technology **Vol 53 No 12 pp 237–245** © IWA Publishing 2006

Introduction

Activated sludge systems involve a myriad of processes interacting in a dynamic environment which usually challenges our engineering ability to optimise, control and maintain a stable treatment performance with respect to effluent quality. To meet these challenges, modelling has been shown to be a useful tool. The IWA series of Activated Sludge Models (ASMs, Henze *et al.*, 2000) represents the most widely accepted and used models for this aim.

One of the important steps in the overall application of models is the selection of an appropriate model structure to describe the biological processes ongoing in the system under study (see Vanrolleghem *et al.*, 2003). The ASM2d of Henze *et al.* (2000), for example, is used to describe process behaviour in enhanced biological phosphorus removing (EBPR) plants carrying out nitrification, denitrification and aerobic COD oxidation processes on top of the phosphorus removal by phosphorus accumulating organisms (PAOs). To maintain an adequate model complexity, however, the ASM2d model had to be based on many simplifying hypotheses and assumptions, e.g. single step nitrification and single step denitrification, among others. These hypotheses however may not be valid for all activated sludge systems, as will be illustrated in detail in this study.

Although some general guidelines are provided to help a modeller choose an appropriate model structure for the activated sludge system under study (Henze *et al.*, 2000; Hulsbeek *et al.*, 2002; Govoreanu *et al.* 2003; Melcer *et al.*, 2003; Langergraber *et al.*, 2004; Vanrolleghem *et al.*, 2003), they tend to be rather simple and, as such, limited to certain types of treatment plant behaviour and performance. Beck (1987), on the other hand, suggests using systems identification tools to ground the development of a model

doi: 10.2166/wst.2006.426

structure on a scientific footing. However, such a tool has not yet been customised for the purpose of activated sludge modelling. In this study, qualitative reasoning is used to develop a model structure. In this approach, the observed systems behaviour, e.g. obtained through dedicated measurement campaign data and long-term daily measurements, is interpreted to find out which biological processes are the most dominating in the system and, hence, need to be included in the model structure that will be chosen or developed.

The main objective of this study is, therefore, to gain insight into the development of appropriate model structures for mechanistic modelling of nitrogen and phosphorus removing activated sludge systems, particularly in SBRs. More specifically, it is aimed at evaluating the ability of a chosen model structure to adequately represent the system subject to changing biological behaviour. To this aim, a pilot-scale SBR receiving a constant wastewater composition and constant influent load was operated using three different operational scenarios. Correspondingly, three measurement campaigns were performed for in-depth monitoring of the dynamics of the process behaviour. To describe the system behaviour, after each measurement campaign an appropriate model structure was developed taking the ASM2d model as a reference model. The results from these three calibrated models are then confronted with reality and evaluated. The BIOMATH protocol (Vanrolleghem *et al.*, 2003) was used to ensure a systematic calibration approach in this study.

Material and methods

The pilot-scale sequencing batch reactor (SBR), described in Insel *et al.* (2006), was operated using two main operating configurations, shown in Figure 1. The influent wastewater used was synthetic. The volumetric exchange ratio (VER), the HRT and the SRT of the SBR were fixed to 0.5, 12 h and 10 d, respectively. The oxygen was controlled using an on-off controller with a dead band (± 0.1) during aerobic react sub-phases. In the last aerobic sub-phase (see Figure 1), the DO set-point was maintained always at 2.0 mgO_2/L in all three operating scenarios, given below in the order of implementation.

First operating scenario

This is also called the reference operation with which the SBR was operated for approximately 2 years. One cycle of this operation is shown in Figure 1 (top). The total volume of the SBR was 80 L and the 40 L of influent was supplied to the reactor at once during the anaerobic-fill phase. The DO set-point was 2 mg/L.

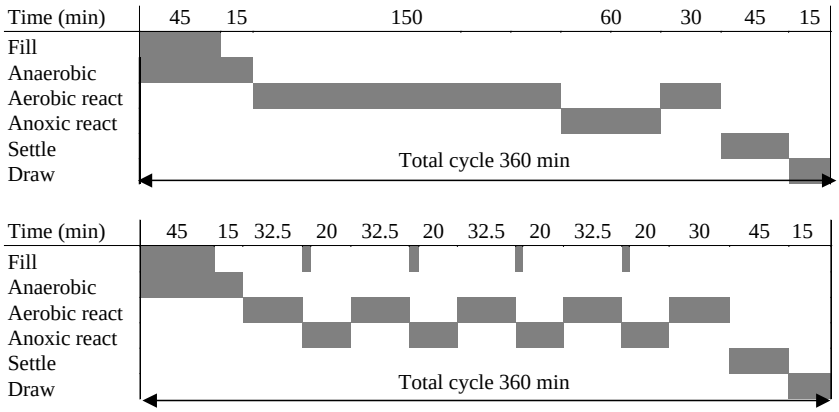

Figure 1 Two operating configurations of the SBR: The reference operating configuration (top), the optimal operating configuration with four aerobic/anoxic sequences (bottom)

Second operating scenario

This scenario, the so-called optimal operation, was found by a systematic model-based study and contains four alternating aerobic and anoxic sub-phases, shown in Figure 1 (bottom). The optimal DO set-point was 0.5 mg/L. The total volume of the SBR was 68 L. Twenty-four litres of the influent was supplied during the anaerobic-fill phase and the remaining 10 L was equally step-fed to the following anoxic phases, i.e. 2.5 L per anoxic phase (see Figure 1 (bottom)).

Third operation scenario

This scenario is in fact the same as the second operation. However, two degrees of freedom of the second operation were changed. First, the DO set-point was increased to 1.0 mg/L and second, the concentrations of the divalent cations (Ca^{2+} and Mg^{2+}) were increased in the influent composition to improve the settling process (Sin *et al.*, 2006b).

All modelling and simulations were performed using WEST® (Hemmis NV, Kortrijk, Belgium).

Results and discussion

The above-mentioned three operating scenarios were implemented in the SBR in the above-mentioned order. The measurement campaigns of the first and the second operations were already described in Insel *et al.* (2006) and Sin *et al.* (2006a), respectively. The third measurement campaign was performed in this study.

Part 1. First operation period: development of the ASM2dN model-structure

The dynamics observed in the SBR obtained during the first operation period are shown in Figure 2 (Insel *et al.*, 2006). In the anaerobic phase, denitrification was completed without nitrite build-up. In this phase, the ammonium concentration only reached approximately 8 mgN/L. Compared to the organic nitrogen present in the reactor, around 30 mgN/L, this level is rather low, indicating a limitation in the hydrolysis/ammonification of the organic

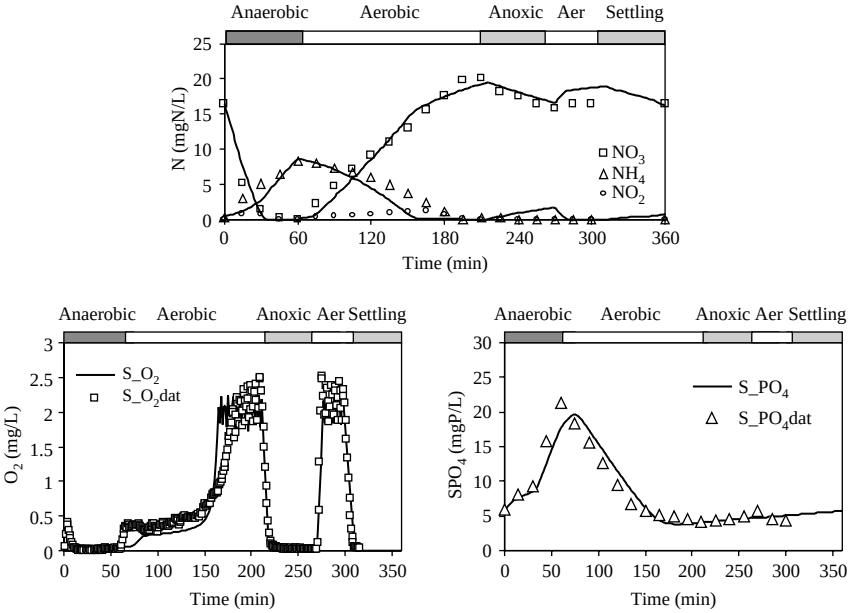

Figure 2 Measured vs. simulated NH_4-N, NO_2-N and NO_3-N (top), oxygen (bottom-left) and phosphate dynamics (bottom-right) with the ASM2dN model (Insel *et al.*, 2006)

Table 1 Summary of the modifications made to the ASM2d model structure in the ASM2dN and ASM2d2N versions (for the complete matrix representation see Sin *et al.* (2004b))

Modified processes	S_{NH}	S_{ND}	S_{NO_3}	S_{NO_2}	S_{N2}	X_{ND}	X_H	X_{NH}	X_{NO}	Kinetic expressions
ASM2dN model (Insel et al., 2006)										
Hydrolysis of entrapped N		1				−1				$\rho_{hydrolysis}\frac{X_{ND}}{X_S}$
Ammonification	1	−1								$k_a S_{ND} X_H$
ASM2d2N model (this study)										
NH_4 oxidation	$-i_{NBM}-1/Y_{NH}$			$1/Y_{NH}$				1		$\mu_{NH}\frac{S_O}{K_{O,NH}+S_O}\frac{S_{NH}}{K_{NH,NH}+S_{NH}}X_{NH}$
NO_2 oxidation	$-i_{NBM}$		$1/Y_{NO}$	$-1/Y_{NO}$					1	$\mu_{NO}\frac{S_O}{K_{O,NO}+S_O}\frac{S_{NO}}{K_{NO2,NO}+S_{NO}}X_{NO}$
NO_3 denitrification	$-i_{NBM}$		$-(1-Y_{HNO_3})/(1.14\ Y_{HNO_3})$	$(1-Y_{HNO_3})/(1.14\ Y_{HNO_3})$			1			$\eta_{NO3,H}\mu_H\frac{K_O}{K_{O,H}+S_O}\frac{S_{NO3}}{K_{NO3,H}+S_{NO3}}\frac{S_{NO3}}{S_{NO2}+S_{NO3}}\frac{S_A}{K_A+S_A}\frac{S_A}{S_F+S_A}X_H$
NO_2 denitrification	$-i_{NBM}$			$-(1-Y_{HNO_2})/(1.72\ Y_{HNO_2})$	$(1-Y_{HNO_2})/(1.72\ Y_{HNO_2})$		1			$\eta_{NO2,H}\mu_H\frac{K_O}{K_{O,H}+S_O}\frac{S_{NO2}}{K_{NO2,H}+S_{NO2}}\frac{S_{NO2}}{S_{NO2}+S_{NO3}}\frac{S_A}{K_A+S_A}\frac{S_A}{S_F+S_A}X_H$
Lysis of X_{NH}									−1	$b_{NH}X_{NH}$
Lysis of X_{NO}								−1		$b_{NO}X_{NO}$

nitrogen. The phosphorus release was observed to be inhibited by the presence of nitrate but reached up to ca 20 mgP/L by the end of the anaerobic phase.

In the subsequent aerobic phase, the nitrification proceeded as one-step and the hydrolysis of the organic nitrogen was observed to proceed, as can be deduced from the nitrogen mass balance in the aerobic phase. Based on these observations, Insel *et al.* (2006) developed the so-called ASM2dN by incorporating the ASM1 hydrolysis and ammonification processes of organic nitrogen into the ASM2d model structure (Henze *et al.*, 2000). This modification is shown in Table 1. It is important to note that the complete matrix representation of these processes is not shown due to space limitations but can be found in Sin *et al.* (2004a,b). The calibrated ASM2dN predictions are also shown in Figure 2. The model simulations are observed to catch the dynamics of nitrogen, phosphorus and oxygen reasonably well.

Part 2. Second operation period: development of the ASM2d2N

Compared to the first operation period (see above), different dynamics were observed, particularly in the nitrogen turnover and the phosphorus concentrations (see Figure 3). First of all, in the anaerobic-fill phase, the NH_4-N is observed to increase up to approximately 18 mgN/L, which indicates the hydrolysis rate of the organic nitrogen is faster than the rate of the first operation.

During the aerobic conditions, NO_2-N was observed to build-up alongside the increasing NO_3-N profile (see Figure 3 (top)), which indicates that the first step of the nitrification process, i.e. ammonia oxidation, occurs faster than the second step, i.e. nitrite oxidation. In the subsequent anoxic conditions, the nitrite and nitrate are observed to be simultaneously denitrified (see Figure 3 (top)) which shows that denitrification occurs using both electron acceptors. The P-release is observed to proceed till the end of the anaerobic phase, reaching about 30 mgP/L (see Figure 3 (bottom)). In the following aerobic conditions, P-uptake took place but in the subsequent anoxic conditions, no P-uptake was observed. On the contrary,

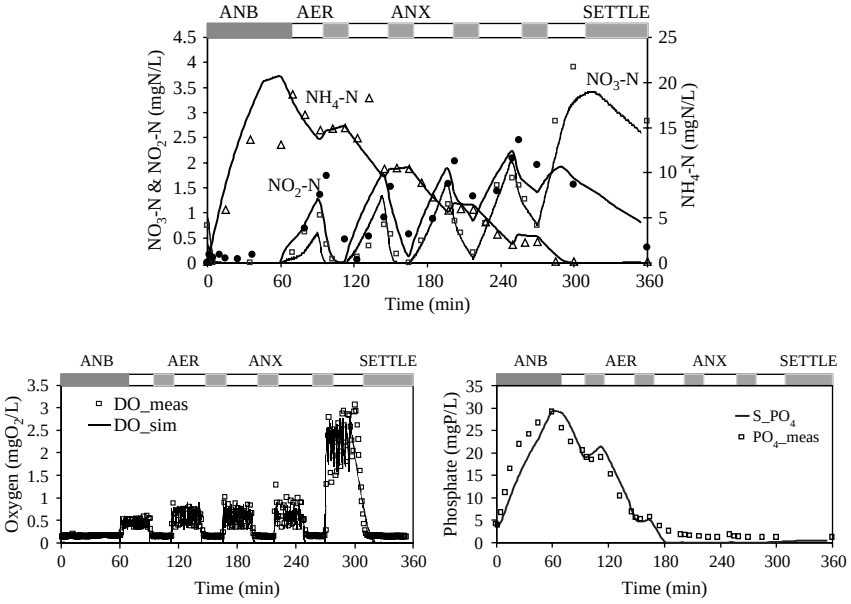

Figure 3 Measured (points) vs. simulated (lines) NH_4-N, NO_2-N and NO_3-N (top), oxygen (bottom-left) and phosphate dynamics (bottom-right) with the ASM2d2N model

Table 2 Summary of the calibrated parameters (indicated in **bold**) of the ASM2dN (Insel *et al.*, 2006) and the ASM2d2N models in the first, second and third operation periods, respectively

Parameters	Description	ASM2dN-1st	ASM2d2N-2nd	ASM2d2N-3rd	Default
Temp	Operating temperature in the SBR	16 °C	23 °C	16 °C	20 °C
$K_{O,NH}$	Saturation coefficient of X_{NH} for oxygen	**0.07**	**0.1**	**0.1**	0.5 mgO_2/L
$K_{O,NO}$	Saturation coefficient of X_{NO} for oxygen	–	**0.3**	**0.3**	0.5 mgO_2/L
$K_{NH,NH}$	Saturation coefficient of X_{NH} for ammonium	1	**0.25**	**0.40**	1 mgN/L
$K_{NH,NO}$	Saturation coefficient of X_{NO} for ammonium	–	**0.05**	**0.1**	1 mgN/L
$K_{O,Het}$	Saturation coefficient of X_H for oxygen	**0.06**	0.2	0.2	0.2 mgO_2/L
$K_{NH,Het}$	Saturation coefficient of X_H for ammonium	**0.01**	0.05	0.05	0.05 mgN/L
$K_{NO3,Het}$	Saturation coefficient of X_H for nitrate	0.5	**0.7**	**0.91**	0.5 mgN/L
$K_{NO2,Het}$	Saturation coefficient of X_H for nitrite	–	0.5	**0.15**	0.5 mgN/L
μ_H	Maximum growth rate of X_H	6	6	**5.1**	6 d^{-1}
μ_{NH}	Maximum growth rate of X_{NH}	**1.5**	**1.05**	**1.1**	1 d^{-1}
μ_{NO}	Maximum growth rate of X_{NO}	–	**1.75**	**1.8**	1 d^{-1}
μ_{PAO}	Maximum growth rate of PAO	**1.8**	**1.8**	1	1 d^{-1}
Q_{PHA}	Rate constant for storage of PHA	**6**	**4.9**	3	3 d^{-1}
Q_{PP}	Rate constant for P-uptake	1.5	**1.7**	1.5	1.5 d^{-1}
$\eta_{NO2,Het}$	Reduction factor for NO_2 denitrification	–	**0.7**	**0.23**	0.8
$\eta_{NO3,Het}$	Reduction factor for NO_3 denitrification	0.8	**0.7**	**0.27**	0.8
K_X	Half saturation constant for hydrolysis	**0.045**	0.1	0.1	0.1
η_{hyd}	Anoxic hydrolysis reduction factor	0.6	**0.7**	**1.0**	0.6
η_{fe}	Anaerobic hydrolysis reduction factor	0.4	**1.0**	**1.0**	0.4
b_{NO}	Decay rate of X_{NO}	–	**0.1**	0.15	0.15 d^{-1}
b_H	Decay rate of X_H	**0.45**	0.4	0.4	0.4 d^{-1}
Y_{HNO2}	Anoxic yield of heterotrophs with NO_2	–	**0.55**	0.63	0.63
Y_{HNO3}	Anoxic yield of heterotrophs with NO_3	**0.58**	0.63	0.63	0.63
i_{NBM}	Nitrogen content of biomass	0.07	**0.086**	**0.073**	0.07
i_{NXI}	Nitrogen content of inert COD	0.02	**0.1**	**0.2**	0.02

phosphorus was slightly increasing probably due to the step-feed of the influent. This implies that the anoxic P-activity is negligible in this SBR reactor.

Confronting the calibrated ASM2dN model with the new dynamics observed in the second operation period led to its falsification (see Sin *et al.*, 2006a). This was not surprising since it was expected that the new established dynamics in the system fall outside the validity range of the ASM2d, i.e. nitrite build-up was assumed negligible in ASM2d. A change in the activated sludge community induced by the second operation was believed to be the underlying reason for this new behaviour reported elsewhere (see Sin *et al.*, 2006b).

To adequately describe the nitrite dynamics in the system, a two-step nitrification model, which is well established in literature (see e.g. Hao *et al.*, 2002) was considered. Yet, modelling the denitrification intermediates under anoxic conditions is not straightforward as there is no unified approach but conflicting theories and assumptions of the reduction pathway for NO_3-N down to N_2 gas exist (Thomsen *et al.*, 1994; Almeida *et al.*, 1995).

However, the following two hypotheses were considered. Hypothesis 1 assumes a parallel denitrification, i.e. $NO_3 \rightarrow N_2$ and $NO_2 \rightarrow N_2$. Hypothesis 2 assumes a sequential denitrification of nitrate down to nitrogen gas, i.e. $NO_3 \rightarrow NO_2 \rightarrow N_2$. These two hypotheses were tested and both provided a good description of the observed behaviour. The problem, in fact, is that the available data were not sufficient to decide which hypothesis holds (Beck, 1987). However, to continue the modelling exercise, hypothesis 2 was selected. The modifications to ASM2d led to the development of the ASM2d2N shown in Table 1.

In Table 2, the calibrated ASM2d2N model parameters are given together with the calibrated parameters of the other two models. The Arrhenius equation was also included in the ASM2d2N to take into account temperature effects. Therefore, the parameters reported in Table 2 correspond to the reference temperature, i.e. 20 °C. The rest of the model parameters were taken default from ASM2d (Henze *et al.*, 2000) and from Hao *et al.* (2002) for the 2-step nitrification model. The predictions of the ASM2d2N model are shown in Figure 3 next to the measurements.

Part 3. Third operation period: Validation of the ASM2d2N model structure

In this period of the SBR operation the oxygen set-point of the second operation was doubled from 0.5 to 1.0 mg/L to improve the activated sludge settling in the system (see Sin *et al.*, 2006b). The resulting response of the SBR to this change is shown in Figure 4. It appears that the bio-P activity of the biomass is lost (Figure 4 (bottom-right)). This is most probably due to inefficient utilisation of the VFA in the influent, which is either oxidised (higher oxygen set-point) or denitrified.

In this operation, the denitrification is clearly observed to occur sequentially, leading to nitrite build-up under anoxic conditions (see the first 45 min in Figure 4 (top)). This information supports the above-mentioned hypothesis 2 that denitrification proceeds via the nitrite route in this SBR. The aerobic nitrite build-up was not pronounced, which is expected since the oxygen stress on the nitrite oxidisers was relieved by the increased oxygen set-point. As for the hydrolysis of organic nitrogen, it is clearly observed to take place in the anoxic conditions too, indicating that hydrolysis is less dependent on the electron acceptor. This is approached by adjusting the reduction factor of the anoxic hydrolysis to 1 (see Table 2).

Although the model structure did not require a modification in this operation period, the model parameters, however, had to be recalibrated, most probably due to the changed behaviour of the biological system.

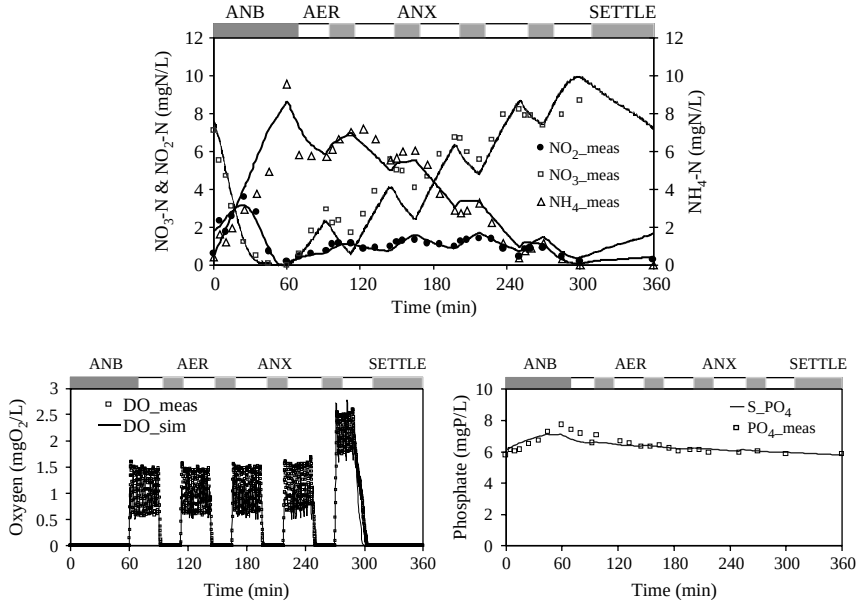

Figure 4 Measured (points) vs. simulated (lines) NH_4-N, NO_2-N and NO_3-N (top), oxygen (bottom-left) and phosphate dynamics (bottom-right) with the ASM2d2N

Critical evaluation of the modified ASM2d models and future perspectives

Although the above-calibrated models were able to catch the dynamics of the system's behaviour to a large extent, still some aspects of it, particularly dealing with the phosphorus removal and anaerobic hydrolysis, could be better described. For example, the fit of ASM2dN to the ammonium profile in the anaerobic phase was different from the observed trajectory (see Figure 2 (top)). Further, the ASM2d2N was clearly limited in predicting the fast rate followed by a decelerated rate in the P-release profile in the anaerobic phase (see Figure 3 (bottom-right)).

The reasons for this discrepancy could be, among others, unobserved system input disturbances, measurement errors, errors in the internal description of the system, i.e. not fully understood biological processes. A system identification approach, as eloquently presented in Beck (1987) and Dochain and Vanrolleghem (2001), may help identification of these discrepancies and therefore contribute to improving the description of the complex behaviour of activated sludge systems.

Conclusions

In this study, the ASM2d was used as a reference model for the description of biological nitrogen and phosphorus removal in a pilot scale SBR. Some of the hypotheses associated with the ASM2d model, hydrolysis of organics nitrogen, nitrite build-up in aerobic and anoxic conditions were observed to become invalid when the systems' behaviour changed. This change was shown elsewhere to be related to a change in the activated sludge community in response to a change in the operation of the system. Therefore, to adequately describe the changed behaviour of the system, the ASM2d had to be modified with new hypotheses such as limited hydrolysis of organic nitrogen, 2-step nitrification and 2-step denitrification. This means that even for the same system receiving a constant influent composition, the ASM2d model structure had to be adapted in response to a change in the system's behaviour.

The modified and calibrated ASM2dN and ASM2d2N were able to well describe nitrogen and oxygen dynamics in the system. However, the prediction of the phosphorus

dynamics remained inadequate. The underlying reasons remain unclear and perhaps would benefit from a system identification approach. Further identifying these discrepancies should help improving modelling of biological phosphorus and nitrogen removal systems.

Acknowledgement

This research was financially supported by the Fund for Scientific Research-Flanders (F.W.O.) and the Ghent University Research Fund. The authors wish to thank Ingmar Nopens, Ruxandra Govoreanu, Dae Sung Lee, Guclu Insel, ChangKyoo Yoo, Kris Villez and Griet Schelstraete for their contribution to the BIOMATH SBR research project. Peter Vanrolleghem is Canada Research Chair in Water Quality Modelling.

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