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A calibration methodology and model-based systems analysis for SBR's removing nutrients under limited aeration conditions

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Abstract
A methodology was proposed for the model calibration of nutrient removing lab-scale SBR's under limited aeration. Based on in-process measurements and influent wastewater characterization, the ASM2d model was modified by adding an organic nitrogen module linked to the hydrolysis mechanism. After calibration the simulation results showed that enhanced biological nutrient removal occurred during the fill-period and under reduced aeration that achieves so-called 'Simultaneous Nutrient Removal'. A model-based systems analysis was performed in terms of the contributions of the different processes to overall oxygen, nitrogen and phosphate utilization. In addition, simultaneously occurring biological reactions were compared during the different phases.

Keywords: SBR, calibration methodology, simultaneous nutrient removal, ASM2dN

INTRODUCTION

Sequencing batch reactors (SBR) are mainly characterized by sequential process phases of fill, react, settle, decant and idle periods that allow considerable flexibility in the design and operation in view of different biological wastewater treatment alternatives (Irvine *et al.*, 1997; Ketchum, 1997). This flexibility is provided by the unique features of SBRs which are: (a) influent and effluent flows are uncoupled by time sequencing (b) the clarification occurs in the same reactor (c) biological processes take place in a cyclic or periodic manner (d) a portion of the treated water is replaced by untreated wastewater for each cycle distinguishing the SBR process from other continuous flow type activated sludge systems (Wilderer *et al.*, 2001; Artan *et al.*, 2001). The design of an SBR for nutrient (nitrogen) removal is mainly based upon the selection of some relevant parameters (e.g. sludge age, volume exchange ratio, cycle time, SVI) as described in, for instance, the ATV guidelines (Teichgräber *et al.*, 2001) in combination with stoichiometric mass balance calculations on the denitrification potential, N_{DP} and available nitrogen, N_A (Artan *et al.*, 2001). In reality, the resulting wastewater treatment plants are mostly over-designed to sustain efficient carbon and nutrient removal under varying environmental and operating conditions. However, attention should be paid to the operating conditions, which may positively or negatively affect the overall system performance, even if the system is designed with safety margins. On the other hand, the optimization of operating parameters (e.g. aeration control) can be an asset to take advantage of simultaneous nitrogen removal together with enhanced biological phosphorous removal known as 'simultaneous nutrient removal' (Daigger and Littleton, 2000).

An existing SBR plant may require a trustable optimization in terms of nutrient removal, but that necessitates better understanding and quantification of the biological processes occurring in each phase. A calibrated activated sludge model is a practical tool to try numerous operation scenarios within a short evaluation time when an upgrade of the SBR is considered (Sin *et al.*, 2003). In this way, the effect of changes in process configuration/control and environmental factors can be simulated and appropriate measures can be taken in due course. However, model calibration requires expert

knowledge on the influent wastewater characterization, on-line/off-line measurements, operating conditions and the treatment system itself. The model-based interpretation of the system than can then be attempted not only leads to better understanding of the biological processes but also provides a way of selecting the most appropriate operating variables to manipulate such as cycle times, aeration capacity *etc.*

In this respect, this paper describes a 'calibration methodology' for a lab-scale SBR performing simultaneous nutrient removal under limited aeration conditions. In addition, a systems analysis is performed via the investigation of individual biological process contributions to phosphate utilization, oxygen consumption and nitrogen removal by using the calibrated model.

MATERIALS AND METHODS

A pilot-scale sequencing batch reactor (SBR) with a working volume of 80 L was seeded with sludge from the Ossemeersen wastewater treatment plant (Gent, Belgium) and operated for a 2 year period. The hydraulic retention time (HRT) and solids retention time (SRT) are maintained at 12 hrs and 10 days, respectively. Each cycle comprises an unaerated fill phase (60 min), aeration phase (150 min), anoxic phase (60 min), aerated phase (30 min), settling (45 min) and draw (15 min) phases. The total cycle time, C_T was set to 6 hours (4 cycles per day) with volumetric exchange ratio (V_0/V_{Total}) of 0.5. The excess sludge is wasted from the end of the aerobic phase for each cycle. A schematic diagram of the SBR system is given in Figure 1. The controls of the duration/sequence of phases and on/off status of peristaltic pumps, mixer and air supply are automatically achieved by a Labview data acquisition and control (DAC) system. The DAC system consists of computer, interface cards, meters, transmitters and solid-state relays. Electrodes for pH, ORP (oxidation-reduction potential), DO (dissolved oxygen), temperature, weight and conductivity are installed and connected to the individual meters. The status of the reactor is displayed on the computer and the time series of the electrode signals are stored in a data log-file. The aeration is controlled by turning on-off the aeration valve. The oxygen is kept around 2 mgO_2/L with an on-off controller with 0.5 mgO_2/L dead band. Synthetic sewage, which mimicks real pre-settled domestic wastewater (Boeije *et al.*, 1998), is used as SBR influent. Based on the model, the influent wastewater characterization in terms of COD fractions, nitrogen and phosphorus components are summarized in Table 1. The measured output variables of ortho-phosphate, dissolved oxygen, ammonia and nitrate nitrogen were used in the calibration study. The volumetric oxygen mass transfer coefficient, K_La, was measured to be 255 d^{-1}. All measurements were carried out according to Standard Methods (APHA, 1998). In the modeling studies, a modification of ASM2d (Henze et al., 1999) was used by the addition of ammonification and hydrolysis of organic nitrogen processes since the influent wastewater contains soluble (0.45 μm) and particulate organic nitrogen that slowly degrade. The settling and decanting phase were characterized by a reactive point-settler model (Kazmi *et al.*, 2001). The simulations were carried out using the WEST simulation package (Vanhooren *et al.*, 2003).

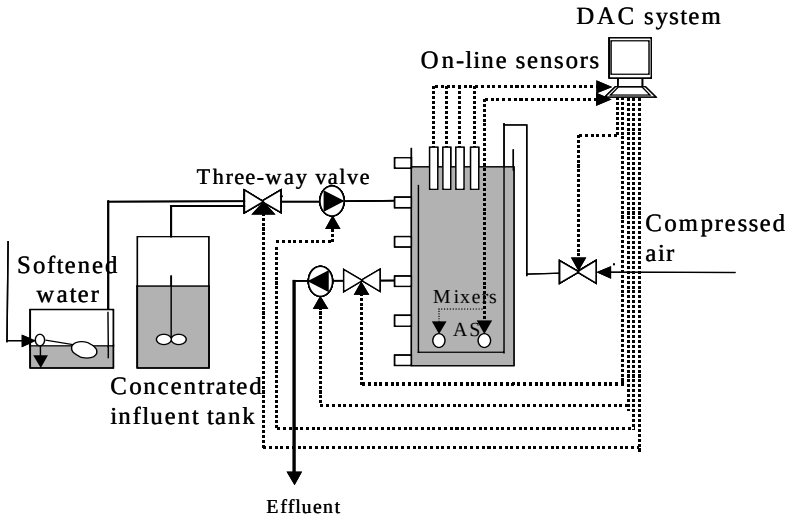

Figure 1. Schematic diagram of the SBR system

Table 1. ASM2dN based influent wastewater characterization (adapted from Boeije *et al.* 1998)

Component	Unit	Concentration	Measurement
Total COD, COD_{tot}	mgCOD/l	411	Lab. analysis
Particulate Inert COD, X_I	mgCOD/l	18	Lab. analysis
Soluble Inert COD, S_I	mgCOD/l	18	Effluent analysis
Biodegradable COD, C_S	mgCOD/l	375	
Fermentable COD, S_F	mgCOD/l	95	Mass balance
Acetate COD, S_A	mgCOD/l	70	GC analysis
Slowly biodegradable COD, X_S	mgCOD/l	210	Mass balance
Ortho-P, S_{PO4}-P	mgP/l	11	Measurement
Total Kjeldahl Nitrogen TKN	mgN/l	63	Lab. analysis
Ammonium nitrogen, NH_4-N	mgN/l	3	Lab. analysis
Soluble biodegradable nitrogen, S_{ND}	mgN/l	10	Mass balance
Particulate biodegradable nitrogen, X_{ND}	mgN/l	50	Mass balance

RESULTS AND DISCUSSION

Measurement campaign results

On-line measurements were performed in the reactor (Figure 2). The nitrification end point, the consumption of nitrate due to denitrification and the phosphate release can be observed from these measurements (Spagni *et al.*, 2001). The corresponding oxygen, O_2, filtered ortho-phosphate, PO_4-P, the nitrate nitrogen, NO_3-N, and ammonia nitrogen, NH_4-N, measurements are presented in Figure 3 and 4. The nitrite nitrogen was found to be negligible. At the beginning of the fill period, a small increase in the oxygen profile occurred because of an inherent oxygen transfer during the feeding and mixing. The gradual pH decrease under anaerobic (filling) conditions can be explained by the net effect of (slow) phosphorus release and denitrification processes. As soon as the consumption of nitrate in the fill phase is completed (Figure 4), a rapid drop in pH can be observed, probably due to fermentation and phosphate release. During the first aerated period, the oxygen concentration is quite low (around 0.3 mg/l) as a result of high oxygen consumption by biomass for readily biodegradable COD degradation with fixed aeration intensity. The effect of CO_2 stripping on the pH profile seems to be higher than that of nitrification up to the mid of the aerated phase (Figure 2). The oxygen concentration increased up to the controlled band of 2±0.5 mgO_2/L. In the following phases, it decreased to zero just after the termination of aeration (Figure 2 right).

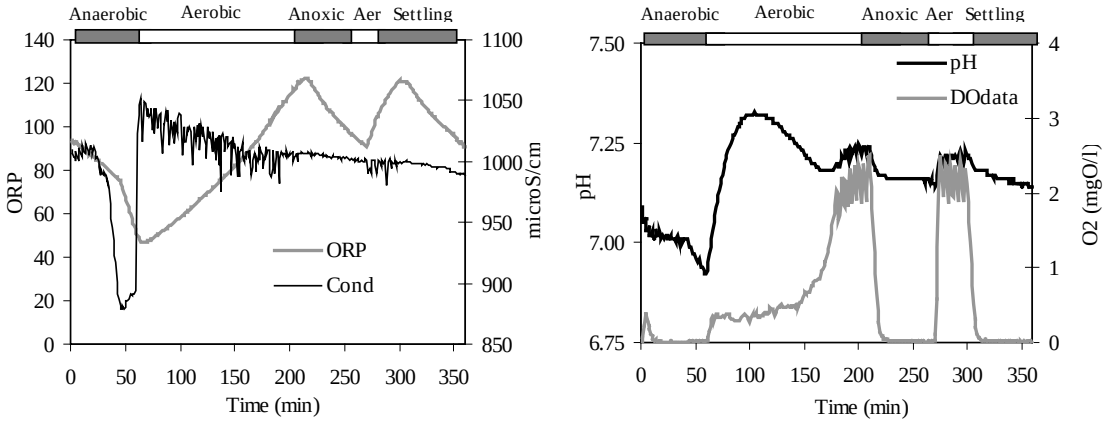

Figure 2. On-line measurements (left) ORP, conductivity and DO, pH (right)

The phosphate concentration increased during the fill phase because of P release (VFA uptake) and filling. Figure 3-right shows that the rate of phosphorus release increased as soon the nitrate was consumed. The remaining VFA was consumed with P-release (Comeau *et al.*, 1990; Kuba *et al.*, 1996). At the end of the first phase, after a steep decline, a gradual increase in the conductivity measurements can be observed after the NO_3 consumption is completed. This can be attributed to phosphorus release

which liberates ions into the bulk. In the aerobic phase, the phosphate is taken up again. There is a slight increase in the phosphate concentration during the 2nd anoxic period probably because of endogenous P-release and COD turnover from the endogenous biomass.

The NH_4-N and NO_3-N profiles are quite interesting in terms of their order of magnitude at the end of the aerobic phase (Figure 4-left). The NO_3 generation is much higher than the observed NH_4-N consumption. This observation reveals that organic nitrogen is transformed into NH_4-N and nitrified to NO_3-N directly and that, in fact, only a net NH_4-N conversion rate is measured. Indeed, after the complete oxidation of NH_4-N, the NO_3-N build-up continues until the end of the first aerobic period. So, the degradation of organic nitrogen becomes the rate-limiting step and must be incorporated in the model in such a way that it is controlled by the hydrolysis mechanism. In the 2nd aerobic period, NO_3-N increased from 17 to 20 mgN/L. The organic nitrogen in the effluent water was measured analytically to be around 1.0 mgN/L which is also in agreement with the simulation result (Figure 4-right). It should be stressed that the total phosphate mass balance resulted in a 98% recovery confirming the exact total sludge age of the system. Within the observation period covering the calibration study, consistent long-term data with respect to effluents together with online measurements shows that the system -under constant conditions- is still at steady state.

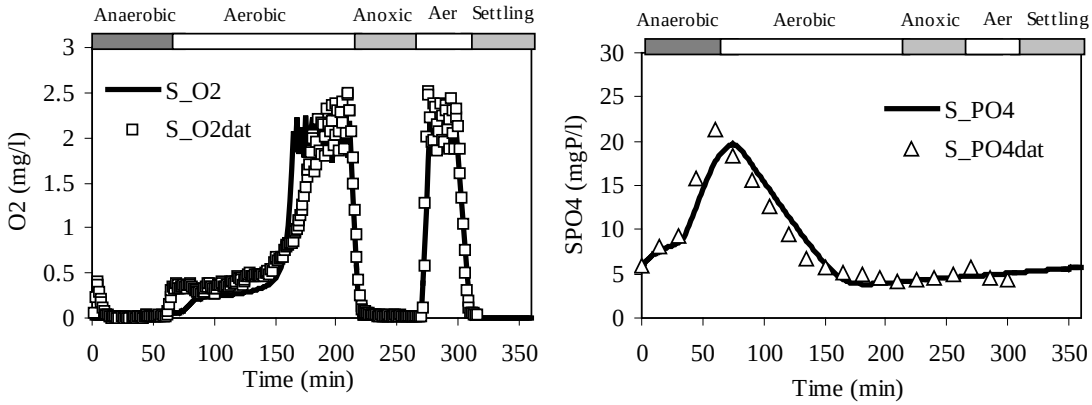

Figure 3. Measurements (symbols) and simulations (lines) of the dissolved oxygen (left) and phosphate (right)

Model selection

The activated sludge model used was built on the basis of ASM1 and ASM2d (Henze *et al.*, 1987; 1999). According to the influent wastewater characterization, the nitrogen transformations were incorporated as an integral module. An approach similar to ASM1 was used. The particulate nitrogen is first hydrolysed to soluble organic nitrogen, S_{ND}, and then ammonified to NH_4-N by heterotrophic biomass.

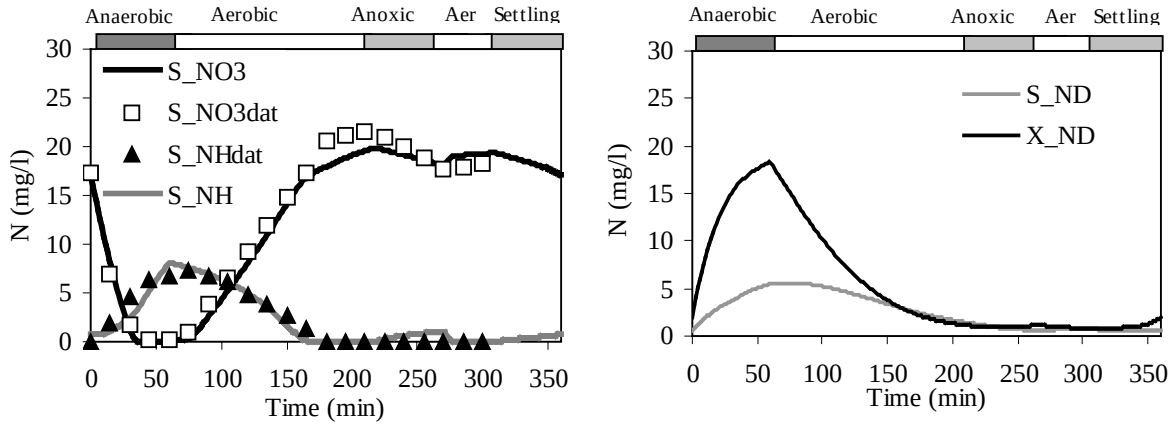

Figure 4. Measurements (symbols) and simulation (lines) of NH_4/NO_3 (left) soluble/particulate nitrogen (right)

The hydrolysis kinetics under anaerobic and anoxic conditions are adapted with correction factors. The kinetics and stoichiometry for autotrophs, the heterotrophs and phosphorus accumulating microorganisms are taken from the ASM2d model except for the anoxic heterotrophic yield, Y_{HNO3}. The default values of the parameters were taken as starting point. The phosphorus components (soluble and particulate) were taken as a fraction of the influent COD fractions and model components. The conservation of the components was calculated according to Gujer and Larsen (1995).

Calibration methodology

A step-wise calibration methodology was developed based on long-term simulations in each iteration step (see Figure 5). As illustrated in Figure 5, a calibration methodology based on expert knowledge was constructed by introducing 4 iterative steps in the order of NH_4-N, O_2 , NO_3-N and PO_4-P profiles, respectively. For each iteration, a 30 day-simulation was carried out to ensure that the state variables gave the same trend in each cycle ("steady state"). The starting point is to obtain the proper activity of the autotrophs to generate NO_3-N. In the first long-term simulation with the default parameter values, the autotrophs were washed out from the system. As a result, the nitrogen half saturation coefficient for autotrophs, K_{NHaut}, was decreased because of the low ammonia concentration in the aerobic phase. Next, the maximum growth rate for autotrophs, $\hat{\mu}_A$, had to be increased in order to sustain autotrophic growth. Later on, the oxygen half saturation constants for autotrophs, $K_{NHaut,}$ and heterotrophs, K_{NH}, were changed to promote heterotrophic growth. In addition, the half saturation constant for hydrolysis, K_X, was included in the calibration to get better fitting of the O_2 profile (Figure 3-left). It should be noted here that each iteration step comprises the preceeding steps to maintain good NH_4-N, O_2, NO_3-N and PO_4-P fits.

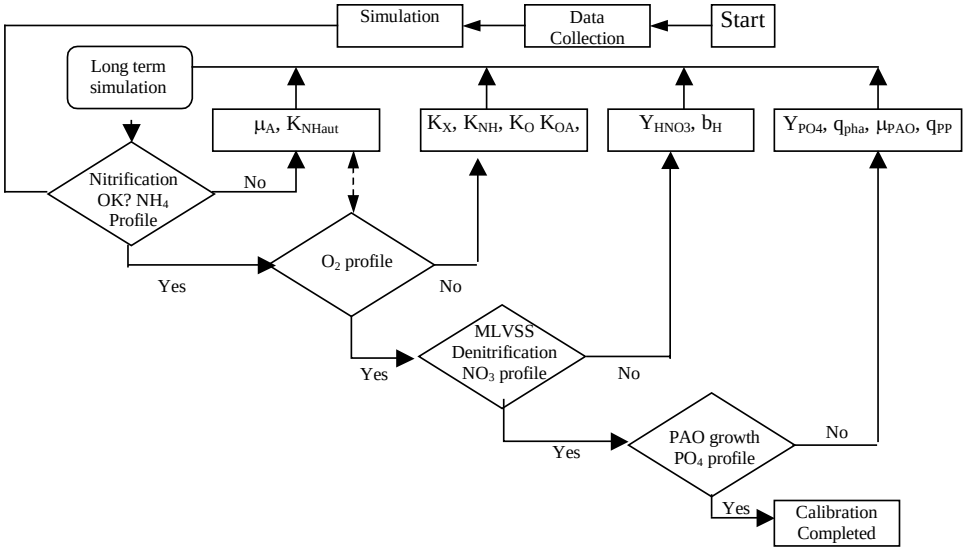

Figure 5. Calibration methodology for the ASM2dN model

In the third step, the anoxic yield was adjusted (0.58 mgCOD/cellCOD) in order to increase the denitrification potential and fit the measured nitrate concentrations. In the literature, the anoxic yield was also reported to be lower than the aerobic yield coefficient (Muller *et al.*, 2003; Orhon *et al.*, 1996). The slope of nitrate during the fill phase was well achieved by the calibration of the heterotrophic lysis rate, b_H. The MLVSS component could be added to Figure 5, but no additional calibration effort was needed for this case. It was measured and simulated around 2000 mg/l. The simulated soluble, S_{ND}, and particulate nitrogen, X_{ND}, profiles are illustrated in Figure 4-right. Finally, the fourth step deals with the calibration of the kinetic constants for the PAOs. The maximum acetate uptake rate of the PAO's, q_{PHA}, had to be increased in order to have them compete successfully with ordinary heterotrophs during the fill phase in the presence of NO_3-N. The reason is that high NO_3-N concentrations during the first 30 minutes of the fill phase caused a high denitrification rate which consumes VFA before the true anaerobic period begins.

Table 2. Summary of the calibrated ASM2dN parameters

Parameter	Unit	Default	Calibrated
Yield coefficient for phosphate release, Y_{PO4}	mgP/mgCOD	0.4	0.38
Anoxic heterotrophic yield, Y_{HNO3}	mgCOD/mgcellCOD	0.63	0.58
Saturation/Inhibition coefficient for O_2, K_O	mgO/l	0.1	0.06
Saturation coefficient for O_2 (autotrophs), K_{OA}	mgO/l	0.5	0.07
Half saturation constant for hydrolysis, K_X	mgCOD/mgcellCOD	0.1	0.045
Endogenous decay rate for heterotrophs, b_H	day^{-1}	0.4	0.45
Rate constant for storage of PHA, q_{PHA}	gCOD/gPP.d	3.0	6.0
Maximum growth rate for PAOs, μ_{PAO}	day^{-1}	1.0	1.8
Maximum growth rate for autotrophs, $\hat{\mu}_A$	day^{-1}	1.0	1.5
Maximum phosphorus storage rate, q_{PP}	gP/gcellCOD.d	1.5	1.3
Half saturation constant for ammonia (heterotrophs), K_{NH}	mgN/l	0.05	0.01
Half saturation constant for ammonia (autotrophs), K_{NHAUT}	mgN/l	1.0	0.2

The yield for phosphate release, Y_{PO4}, had to be decreased to fit the fill-phase PO_4-P profile. As stated in the ASM2d model, the storage compound, X_{PHA}, is consumed by two simultaneous processes, i.e. the phosphate uptake and the growth of PAOs. During calibration, the concentration of X_{PAOs} was increased by adjusting the maximum growth rate of PAOs, $\hat{\mu}_{PAO}$, to a higher value. Meanwhile, to achieve steeper slope and also to reach the constant PO_4 concentration at the end of the aerobic phase, the maximum phosphate uptake rate, q_{PP}, was increased (Figure 2-left). The calibration task was terminated when the simulated profiles were closest to all measured data (see Figure 2-4). The values of the calibrated parameters together with their default values are listed in Table 2.

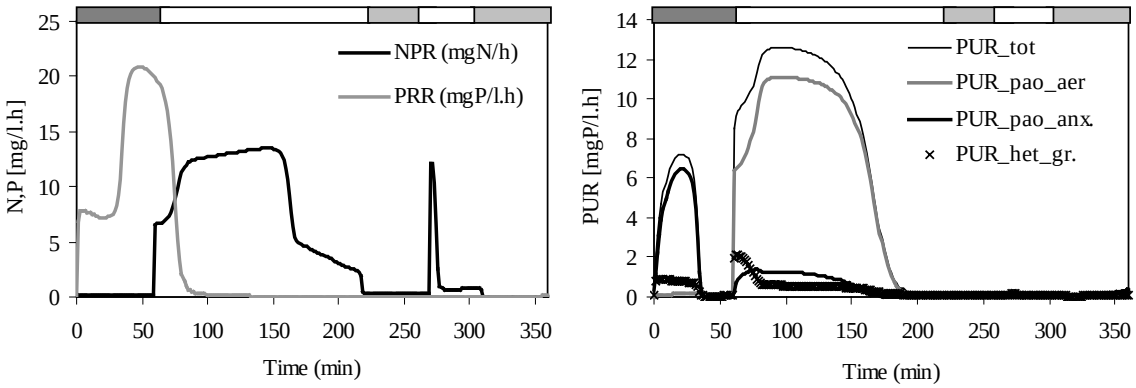

Figure 6. Nitrate production, P-release (left) and segments of phosphate utilization rate (right)

Systems analysis

Using the calibrated model, the trajectories of the process rates were drawn to visualize the contribution of each process to the overall SBR behaviour. It is obvious from Figure 6-left that the P-release rate after the mid of the fill phase is 2.5 times higher (21 mgP/l.h) than that at the beginning of the phase (7.5 mgP/l.h) because of the removal of NO_3-N. This continues until the external carbon source is consumed completely after around 100 min and the oxygen concentration increases. The nitrate production rate, NPR, immediately increased when aeration is turned on. The rate dropped from 13 mgN/l.h to around 5 mgN/l.h when it became hydrolysis limited. The simulation for the total phosphate utilization rate, PUR, reveals that the maximum contribution pertains to the aerobic phosphate uptake by the PAOs (73% of the overall P uptake) initially exhibiting an uptake rate of 11 mgP/l.h (Figure 6-right). As can be observed from Figure 6-right and Figure 7, P-release, anoxic P-uptake and VFA storage took place simultaneously. It is important to mention here that 19% of the removed P is taken up by the PAOs anoxically during the fill phase (12%). In the aerobic phase 7% of P is removed (Figure 8). The rate of the anoxic P uptake at the start of the aerobic phase was simulated to be around 1.4 mgP/l.h. The P uptake via heterotrophic growth only covers 8% of the overall P-removal (growth of nitrifiers is neglected).

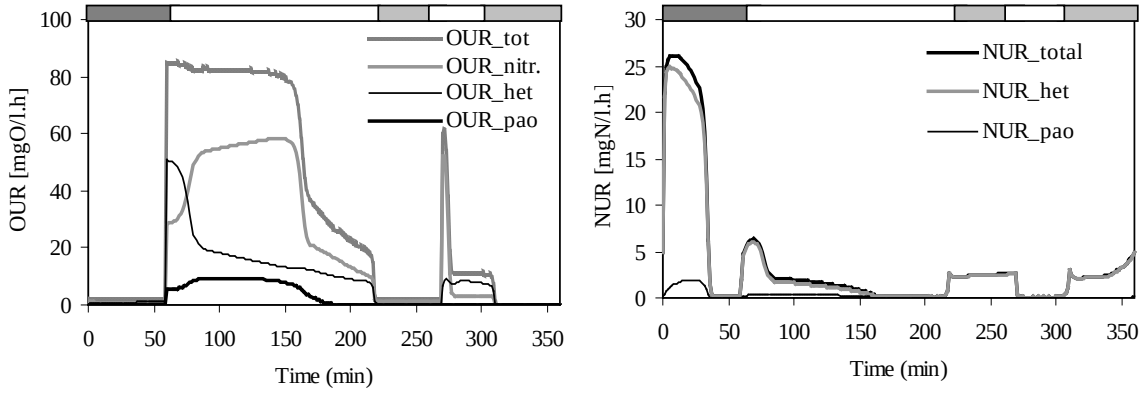

Figure 7. OUR and NUR contributions in a SBR cycle

According to the simulation results, the distribution of denitrified nitrogen over each of the phases can be summarized as follows: (a) 61% of total denitification took place in the first phase (fill phase), (b) 17% was denitrified under aerobic conditions due to simultaneous nitrification-denitrification (Münch *et al.*, 1996), (c) 10% denitrification was achieved in the 2nd anoxic period and (d) 10% denitrification in the settling phase. The simulation based calculations showed that 22 mg/L NO_3-N was denitrified in one cycle which is comparable with the denitrification potential calculation performed according to Artan *et al.* (2001) which led to a value of 18 mgN/l. This difference can be explained as follows. First, it should be acknowledged that the 22 mg/L does not regard the denitrification potential used by the PAOs. Another point is the additional denitrification in the aerobic phase due to low oxygen levels. This is not considered in the stoichiometric calculation. The nitrate utilization rate, NUR, is mainly governed by ordinary heterotrophic activity, i.e. 89% of the total denitrified nitrogen is used up by these microorganisms. Only 11% is consumed in denitrifying PAO activity (Figure 7- right).

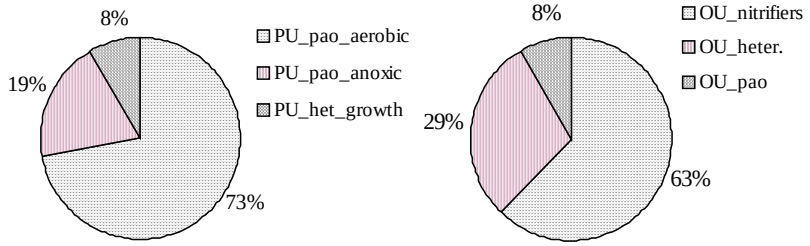

Figure 8. The phosphate and oxygen utilization in one SBR cycle

The maximum total oxygen uptake rate, OUR, is around 82 mgO_2/l.h until 150 min (nitrification end point) and is governed by the oxygen transfer capacity. Within the aerobic phase, the maximum oxygen uptake rates for the autotrophs, heterotrophs and PAOs are around 50, 50 and 10 mgO_2/l.h, respectively. However these maximum rates are reached in different periods of the aerobic phase (see Figure 7). The distribution of cumulative oxygen consumptions over the processes is given in Figure 8-right. The autotrophic biomass accounts for 63% of the total oxygen consumption of the system. The ordinary heterotrophs only consume 29%.

CONCLUSIONS

A systematic model calibration methodology was applied successfully to a lab-scale SBR exhibiting simultaneous nitrification-denitrification together with biological phosphorus removal, the so-called ‘simultaneous nutrient removal’. The biological processes described in the model were found to occur simultaenously under limited aeration conditions. A low oxygen transfer inherently differentiates the system behaviour from systems under traditional design calculations. As a result, the oxygen transfer

should strictly be incorporated in the calibration of biological nutrient removal to visualize the individual contributions of each process. From this point of view, models may serve as practical tools to evaluate alternatives for the optimization of SBR's. The stepwise calibration methodology applied here is necessary for an effective selection of the relevant parameters to be calibrated.

The systems analysis performed with the calibrated model clearly illustrated that the denitrification at the start of the aerobic phase and during the settling phase has a considerable contribution to the overall denitrification capacity of the system and also affects biological phosphate removal. It therefore warrants further study.

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REFERENCES

APHA (1998) *Standard Methods for the Examination of Water and Wastewater*, 20th ed. American Public Health Association, Washington DC.

Artan N., Wilderer P., Orhon D., Morgenroth E. and Özgür N. (2001) The mechanism and design of sequencing batch reactor systems for nutrient removal-the state of the art. *Wat. Sci. Tech.*, **43**(3), 53-60.

Boeije G., Corstanje R., Rottiers A. and Schowanek D. (1998). *Adaptation of the CAS test systemand synthetic sewage for biological nutrient removal. Part I: Development of a new syntheticsewage.* Chemosphere, **38**(4), 699-709.

Comeau Y., Hall KJ. and Oldham, K. (1990) Indirect phosphate quatification in activated sludge. *Water Pollut. Res. J. Canada*, **25**(2), 161-174.

Daigger G.T. and Littleton H.X. (2000) Characterization of simultaneous nutrient removal in staged, closed-loop Bioreactors. *Water Env. Res.*, 72(3), 330-339.

Gujer W. and Larsen T.A. (1995) The implementation of biokinetics and conservation principles in ASIM. *Wat. Sci. Tech.*, **31**(2): 257-266.

Henze M., Grady C.P.L.Jr., Gujer W., Marais G.v.R. and Matsuo T. (1987) *Activated Sludge Model No.1*, IAWPRC Science and Technical Report No. 1, IAWPRC, London.

Henze M., Gujer W., Mino T., Matsuo T., Wentzel M.C., Marais G.V.R. and Van Loosdrecht M.C.M. (1999) Activated Sludge Model No.2d, ASM2d, *Wat. Sci. Tech.*, **39**(1), 165-182.

Irvine R.L., Wilderer P.A. and Flemming H.C. (1997) Controlled unsteady state processes and technologies-an overview. *Wat. Sci. Tech.*, **35**(1), 11-18.

Kazmi A.A., Fujita M. and Furumai H. (2001) Modeling effect of remaining nitrate on phosphorus removal in SBR. *Wat. Sci. Tech.*, **43**(3), 175-182.

Ketchum L.H.Jr. (1997) Design and physical features of sequencing batch reactors. *Wat. Sci. Tech.*, **35**(1), 1-10.

Kuba T., Wachtmeiser A., van Loosdrecht M.C.M. and Heijnen J.J. (1994) Effect of nitrate on phosphorus release in biological phosphorus removal systems. *Wat. Sci. Tech.*, **30**(6), 263-269.

Muller A., Wentzel M.C., Loewenthal R.E. and Ekama G.A. (2003) Heterotrophic anoxic yield in anoxic aerobic activated sludge systems treating municipal wastewater. *Wat. Res.*, **37**(10), 2435-2441.

Münch E.V., Lant P. and Keller J. (1996) Simultaneous nitrification and denitrification in bench-scale sequencing batch reactors. *Wat. Res.*, **30**(2), 277-284.

Orhon D., Sözen S. and Artan N. (1996) The effect of heterotrophic yield on the assessment of the correction factor for anoxic growth. *Wat. Sci. Tech.*, **34**(5-6), 67-74.

Sin G., Insel G., Lee D.S. and Vanrolleghem P.A. (2003) Optimal but robust N and P removal in SBRs: A systematic study of operating scenarios. *3rd IWA international Conference on SBRs*, Queensland, Australia (submitted).

Spagni A., Buday J., Ratini P. and Bortone G. (2001) Experimental considerations on monitoring ORP, pH, conductivity and dissolved oxygen in nitrogen and phosphorus biological removal processes. *Wat. Sci. Tech.*, **43**(11), 197-204.

Teichgräber B., Schreff D., Ekkerlein C. and Wilderer P.A. (2001) SBR technology in Germany - An overview. *Wat. Sci. Tech.*, **43**(3), 323-330.

Vanhooren H., Meirlaen J., Amerlinck Y., Claeys F., Vangheluwe H. and Vanrolleghem P.A. (2003) WEST: Modeling biological wastewater treatment. *J. Hydroinformatics*, **5**, 27-50.

Wilderer P., Irvine RL., Goronszy M.C. (2001) *Sequencing Batch Reactor Technology*, IWA Scientific and Technical Report No:10, London.