Benchmarking biological nutrient removal in wastewater treatment plants: influence of mathematical model assumptions

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ABSTRACT

This paper examines the effect of different model assumptions when describing biological nutrient removal (BNR) by the activated sludge models (ASM) 1, 2d & 3. The performance of a nitrogen removal (*WWTP1*) and a combined nitrogen and phosphorus removal (*WWTP2*) benchmark wastewater treatment plant was compared for a series of model assumptions. Three different model approaches describing BNR are considered. In the reference case, the original model implementations are used to simulate *WWTP1* (ASM1 & 3) and *WWTP2* (ASM2d). The second set of models includes a reactive settler, which extends the description of the non-reactive TSS sedimentation and transport in the reference case with the full set of ASM processes. Finally, the third set of models is based on including electron acceptor dependency of biomass decay rates for ASM1 (*WWTP1*) and ASM2d (*WWTP2*). The results show that incorporation of a reactive settler: (1) increases the hydrolysis of particulates; (2) increases the overall plant's denitrification efficiency by reducing the S_{NOx} concentration at the bottom of the clarifier; (3) increases the oxidation of COD compounds; (4) increases X_{OHO} and X_{ANO} decay; and, finally, (5) increases the growth of X_{PAO} and formation of $X_{PHA,Stor}$ for ASM2d, which has a major impact on the whole P removal system. Introduction of electron acceptor dependent decay leads to a substantial increase of the concentration of X_{ANO}, X_{OHO} and X_{PAO} in the bottom of the clarifier. The paper ends with a critical discussion of the influence of the different model assumptions, and emphasizes the need for a model user to understand the significant differences in simulation results that are obtained when applying different combinations of 'standard' models.

Key words | ASM1, ASM2d, ASM3, activated sludge model, benchmarking, electron acceptor dependent decay, reactive settler

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NOMENCLATURE

AER	aerobic section
ANAER	anaerobic section
ANOX	anoxic section
ASM1	Activated Sludge Model no. 1
ASM2d	Activated Sludge Model no. 2d
ASM3	Activated Sludge Model no. 3
COD	chemical oxygen demand
K_La	volumetric oxygen transfer coefficient (days^{-1})
Q_{INTR}	internal recycle flow rate ($m^3 \cdot day^{-1}$)
Q_R	external recirculation flow rate ($m^3 \cdot day^{-1}$)
Q_W	waste flow rate ($m^3 \cdot day^{-1}$)
S_B	biodegradable substrate ($g\ COD \cdot m^{-3}$)
S_F	fermentable organic matter ($g\ COD \cdot m^{-3}$)
S_{NHx}	ammonium plus ammonia nitrogen ($g\ N \cdot m^{-3}$)
S_{NOx}	nitrate plus nitrite nitrogen ($g\ N \cdot m^{-3}$)
S_{O2}	dissolved oxygen ($g\ -COD \cdot m^{-3}$)
S_{PO4}	soluble inorganic phosphorus ($g\ P \cdot m^{-3}$)
S_{VFA}	fermentation products, considered to be acetate ($g\ COD \cdot m^{-3}$)
TSS	total suspended solids ($g \cdot m^{-3}$)
X_{ANO}	autotrophic nitrifying organisms ($g\ COD \cdot m^{-3}$)
X_{OHO}	heterotrophic organisms ($g\ COD \cdot m^{-3}$)

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X_{PAO} phosphorus accumulating organisms ($g\ COD \cdot m^{-3}$)
$X_{PAO,Stor}$ cell internal storage product of phosphorus accumulating organisms ($g\ COD \cdot m^{-3}$)
X_U particulate non-degradable organics ($g\ COD \cdot m^{-3}$). The origin of the compound in ASM1 is specified by E (endogenous process) and inf (influent)
XC_B slowly biodegradable substrate ($g\ COD \cdot m^{-3}$)
WWTP1 benchmark simulation layout no. 1 (carbon and nitrogen removal)
WWTP2 benchmark simulation layout no. 2 (carbon, nitrogen and phosphorus removal)

RESEARCH HIGHLIGHTS

- ASM1, ASM2d and ASM3 were extended with: (1) reactive settler and (2) electron acceptor decay dependency.
- Biological nutrient removal was evaluated by means of two different wastewater treatment plants (*WWTP1* & *2*) using the previously defined model assumptions.
- A reactive settler model dramatically increases the overall plant's denitrification efficiency. The latter has a paramount importance when bio-P processes are involved.
- Electron acceptor decay dependency offers a more realistic process description, particularly when a reactive settler is considered, decreasing the massive biomass death due to the extra biological volume.

INTRODUCTION

Activated sludge models (ASMs) are widely used for benchmarking (Copp 2002; Jeppsson *et al.* 2007; Nopens *et al.* 2010), diagnosis (Rodriguez-Roda *et al.* 2002), design (Flores *et al.* 2007; Benedetti *et al.* 2010), teaching (Hug *et al.* 2009) and optimization (Rivas *et al.* 2008) of wastewater treatment plants (WWTPs). The ASM family (Henze *et al.* 2000) successfully describes the biochemical removal of organic carbon (C), nitrogen (N) and phosphorus (P) and can be considered as reference models. Continuous research is still carried out in order to extend these models, for example by including additional processes, with the purpose of improving biological nutrient removal (BNR) predictions and explaining other aspects of the processes. Some of these recent developments are: pH calculation (Serralta *et al.* 2004), two-step nitrification-denitrification (Iacopozzi *et al.* 2007; Sin *et al.* 2008), four-step denitrification (Hiatt & Grady 2008), the inclusion of toxic compounds (Copp & Spanjers 2004; Rosen *et al.* 2008) and the effect of microbiology-related TSS separation problems (Hug *et al.* 2006; Flores-Alsina *et al.* 2009).

In order to obtain proper simulation results for a specific WWTP, several studies have focused on developing standardized procedures for calibrating ASMs (Hulsbeek *et al.* 2002; Petersen *et al.* 2002; Melcer *et al.* 2003; Langergraber *et al.* 2004; Gillot *et al.* 2009; Corominas *et al.* 2011), efforts that have also resulted in the formation of the IWA Task Group on Good Modelling Practice (GMP). Even though the GMP protocol together with older protocols includes a stage that is dedicated to model selection, the implications of different model assumptions resulting in changes in the model structure have not been thoroughly compared in the three most widespread ASM implementations, i.e. ASM1, 2d and 3. Paying attention to model selection and model assumptions is important, especially in view of the fact that the ASM models triggered the general acceptance of WWTP modelling, first in the research community and later on also in engineering consultancy.

The Benchmark Simulation Model (BSM) platform has been widely used in both academia and industry for unbiased comparison of control strategies (Copp 2002). The original activated sludge configuration of the BSM1 has for example been upgraded for other plant configurations (Gernaey & Jørgensen 2004; Pons & Potier 2004). In addition, the BSM1 was adapted for long-term evaluation (Rosen *et al.* 2004), and has been extended with additional units, resulting in a plant-wide simulation benchmark, the BSM2 (Jeppsson *et al.* 2007; Nopens *et al.* 2010). In this manuscript, the BSM platform was used to examine the effects of different model assumptions when describing the BNR processes considered by the ASM1, 2d & 3. The differences when adding a reactive settler and electron acceptor dependent decay rates to the original ASM implementations are compared using two benchmark WWTPs. The simulation results are complemented with a rigorous analysis of soluble and particulate compounds in both the sludge blanket and the effluent. The paper is organized as follows: First, the two benchmark WWTP designs and operational conditions are presented. Next, the investigated set of different modelling approaches is described. Finally, a critical discussion of the results and a summary of the main conclusions are given.

METHODS

WWTPs under study

Two benchmark WWTPs are considered in this study. First, a N removal plant (*WWTP1*) consisting of five reactors in series and one secondary sedimentation tank (SEC) is investigated. Tanks 1 and 2 are anoxic (ANOX1 and 2) and have a total volume of 2,000 m^3. Tanks 3, 4 and 5 (AER1, 2 and 3) are aerobic with a total volume of 4,000 m^3. AER3 and ANOX1 are linked by means of an internal recycle (Q_{INTR}). A default open loop control strategy is defined based on the following values: K_La (AER1, 2 & 3) = 240, 240 and 84 day^{-1} (aeration intensity, represented as the volumetric oxygen transfer coefficient), $Q_R = 18{,}446\ m^3 \cdot day^{-1}$ (external recirculation) and $Q_W = 385\ m^3 \cdot day^{-1}$ (wastage flow rate). Further information about design and operational characteristics can be found in Copp (2002). Secondly, a combined N and phosphorus (P) removal plant (*WWTP2*) is studied, where two additional anaerobic reactors (ANAER1, 2) with a total volume of 2,000 m^3 are added in front of *WWTP1*. The *WWTP2* plant has the same operational settings as *WWTP1*. The secondary settler of both *WWTP1* and *WWTP2* has a surface area of 1,500 m^2 and a total volume of 6,000 m^3. The two plant layouts are presented in Figure 1.

Mathematical models

Three sets of model assumptions describing BNR processes are compared:

- In the reference case, the ASM1 and ASM3 (Henze *et al.* 2000) are chosen to describe the biological processes in *WWTP1*, while for *WWTP2* the selected model is the ASM2d (Henze *et al.* 2000). Kinetic and stoichiometric parameters are defined for 15 °C and are reported in Henze *et al.* (2000). In all cases the double-exponential velocity function of Takács *et al.* (1991) is used to model the secondary settling process through a one-dimensional non-reactive 10-layer settler. Parameters can be found in Copp (2002).
- The second set of models forms an extension of the reference case, upgrading the description of the TSS sedimentation and transport in the settler with the full set of ASM1, ASM3 (*WWTP1*) and ASM2d (*WWTP2*) equations using the reactor kinetic and stoichiometric parameters, i.e. introducing reactive settlers (Gernaey *et al.* 2006).

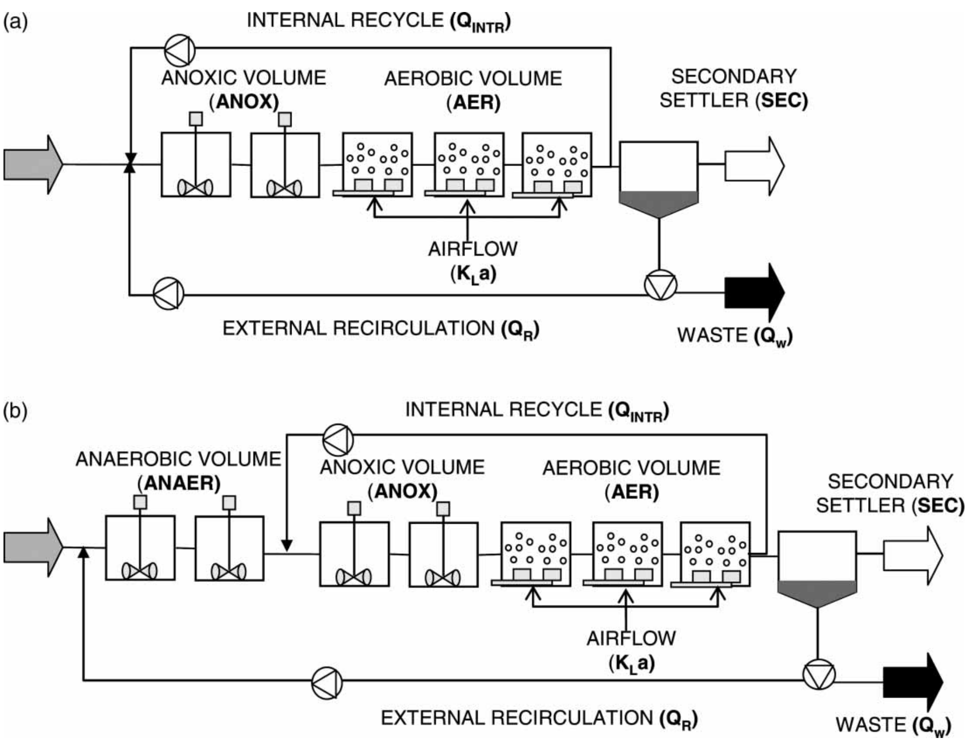

Figure 1 | *WWTP1*: organic carbon and nitrogen removal plant (a) and *WWTP2*: organic carbon, nitrogen and phosphorus removal plant (b).

- Finally, the third set of models is based on extending ASM1 (*WWTP1*) and ASM2d (*WWTP2*) with biomass decay rates that are electron acceptor dependent. Default parameters can be found in Gernaey and Jørgensen (2004). In this case, ASM3 (*WWTP1*) is not modified because it already includes the possibility to differentiate the decay rates of heterotrophs and autotrophs under aerobic and anoxic conditions.

A 28 day influent profile was generated following the principles outlined in Gernaey *et al.* (2011). All plant models are subjected to identical influent flow rate and pollutant loads in terms of COD and N (P added to *WWTP2* input as well). Simulation results were evaluated dynamically during the last seven days of simulation in accordance with BSM1 principles (100 days simulation to reach steady state, then 28 days of dynamic influent data). Only the last seven days of data are used for evaluation.

BNR PERFORMANCE WITH REACTIVE SETTLER (ASM1, 2d AND 3)

Underflow results

Figures 2 and 3 show the steady state values of the soluble (S) and particulate (X, XC) compounds when the *WWTP1* and *WWTP2* are simulated for the different model assumptions. When ASM1, 2d and 3 processes are implemented in the secondary settler model (model assumption set number two), there are substantial differences in the behaviour of the soluble components (*S*) compared to the reference case (non-reactive secondary settler). The S_{O2} concentration decreases rapidly towards the bottom of the clarifier (layer 6–10), thus increasing the overall denitrification efficiency (layer 9–10), i.e. the S_{NOx} concentration is reduced in the reactive settler using S_B as substrate (see S_{O2}, S_{NOx} and S_B profiles in Figure 2). Figure 2 also shows

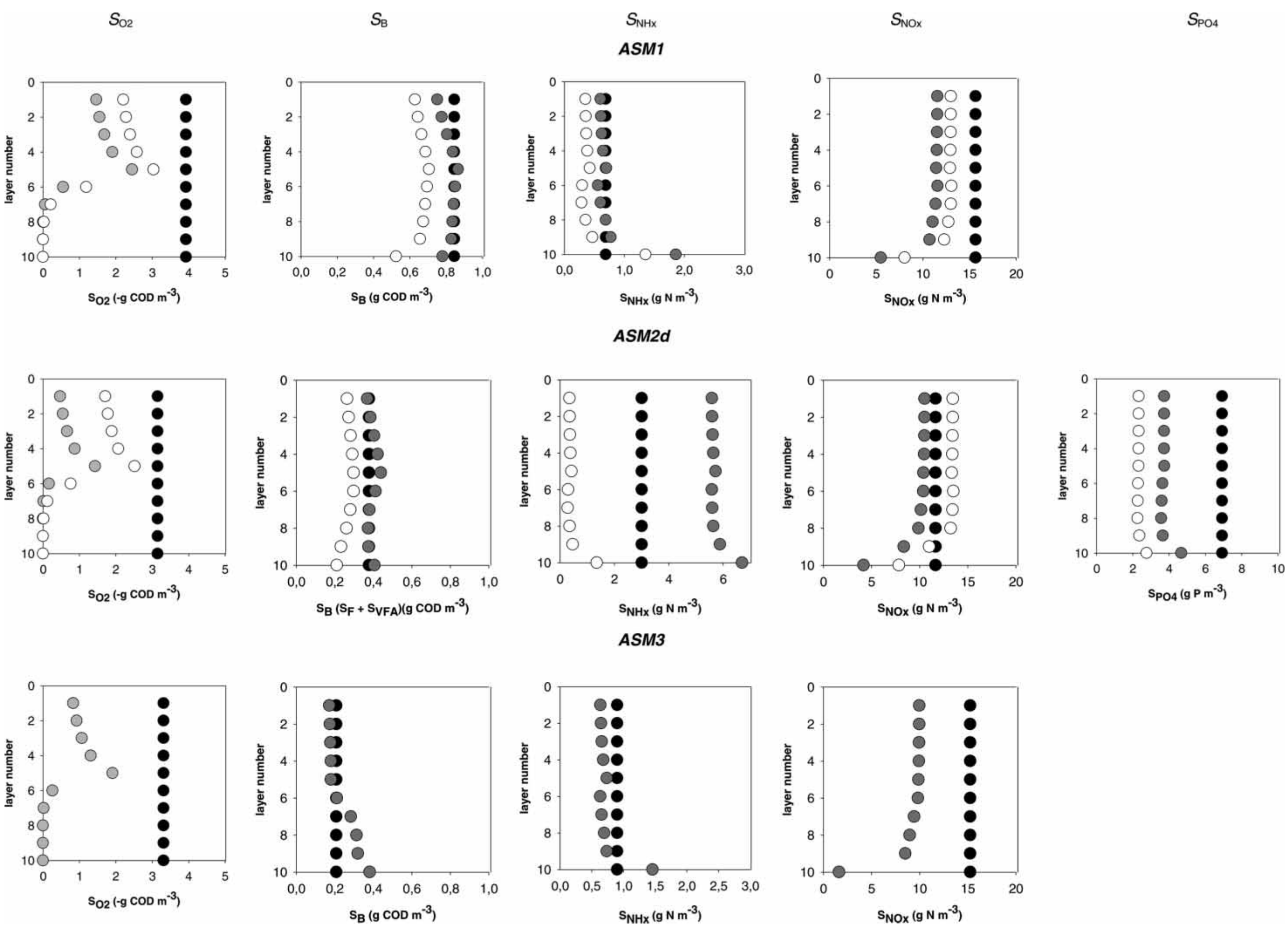

Figure 2 | S_{O2} (first column), S_B (second column), S_{NHx} (third column), S_{NOx} (fourth column) and S_{PO4} (fifth column) concentrations in the different layers of the settler for ASM1 (first row), ASM2d (second row) and ASM3 (third row). The different modelling concepts are colour coded: black (default), grey (reactive settler) and white (reactive settler + decay modification).

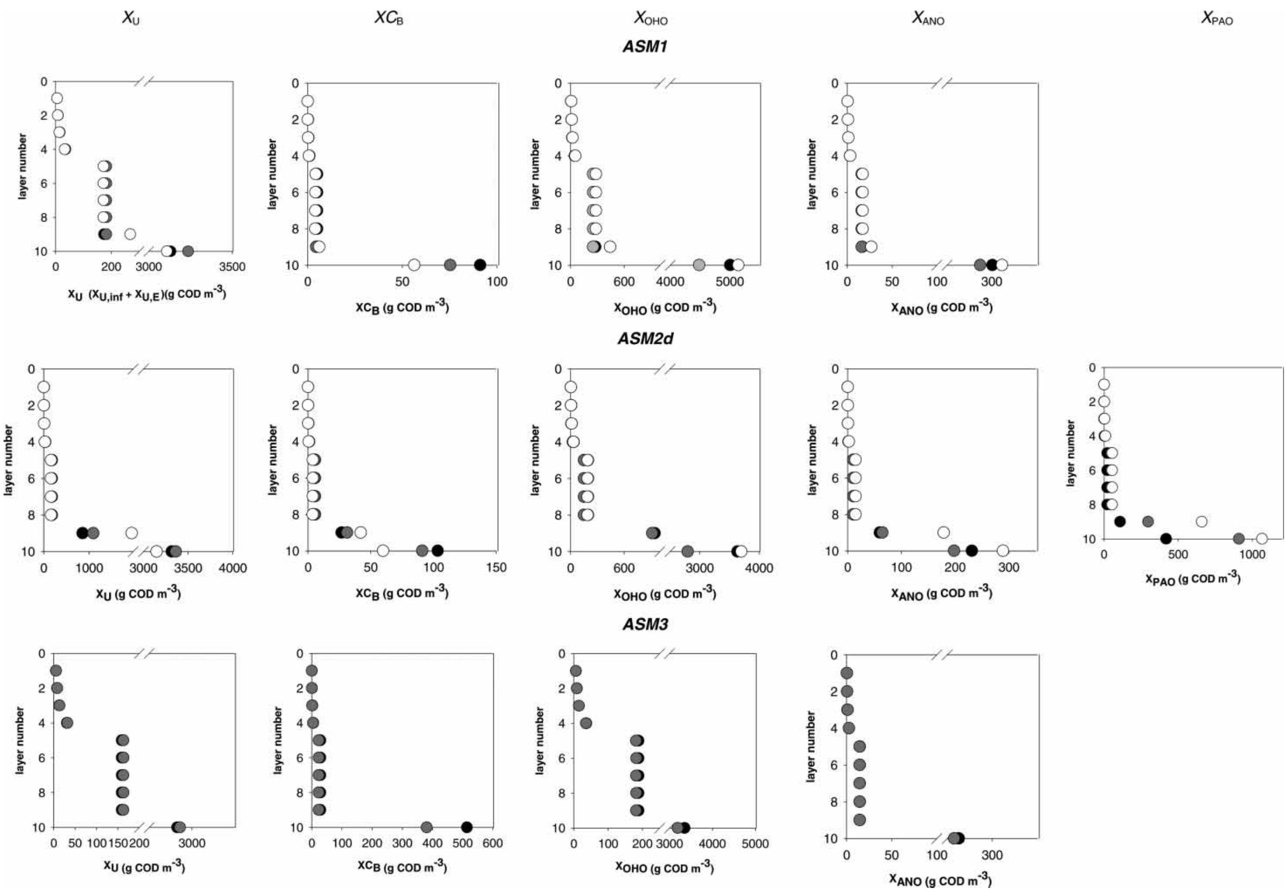

Figure 3 | X_U (first column), XC_B (second column), X_{OHO} (third column), X_{ANO} (fourth column) and X_{PAO} (fifth column) concentrations in the different layers of the settler for ASM1 (first row), ASM2d (second row) and ASM3 (third row). The different modelling concepts are colour coded: black (default), grey (reactive settler) and white (reactive settler + decay modification).

a slight increase of the underflow concentrations of S_{NHx} and S_{PO4}, mainly due to increased hydrolysis and S_{PO4} release (S_{PO4} only in ASM2d). The fate of the particulate XC_B, X_U, X_{OHO}, X_{ANO} and X_{PAO} components in the settler was also investigated with and without reactive settler. In both *WWTP1* and *2*, the XC_B fraction does not change too much at the feed point (layer 5) and towards the top (layer 1–4). However, it decreases towards the bottom (layer 6–10) of the clarifier in the reactive settler as a result of hydrolysis. Moreover, X_{OHO} and X_{ANO} concentrations decrease at the bottom of the clarifier due to a higher decay rate, i.e. death of heterotrophic and autotrophic organisms is considered during the settling phase. Therefore, there is an increase of X_U (see Figure 3). Finally, for ASM2d (*WWTP2*), it can be observed that the X_{PAO} concentration is dramatically increased when including the reactive settler (Figure 3). This situation is mainly due to the lower quantity of S_{NOx} returned via the internal recycle flow to ANAER1. Therefore, there is a higher P uptake because the readily biodegradable substrates (S_F and S_{VFA}) entering the WWTP are now increasingly used to create cell internal $X_{PAO,Stor}$ (the concentration of this component also increases) instead of being used by X_{OHO} with S_{NOx} as electron acceptor.

Overflow results

Compared to the reference case, the simulation results show that there is an increase of the effluent S_{NHx} concentration in ASM2d (*WWTP2*) reactive settler implementations (Figure 2). This fact is attributed to the introduction of autotrophic decay in the lower layers of the settler, i.e. X_{ANO} biomass dies and does not grow due to the anoxic conditions at the bottom of the secondary settler, also because decay does not depend on the type of electron acceptor present in ASM2d. The latter also affects the effluent S_{NOx} concentration, which is lower for the simulation with the reactive settler. Most probably it is caused by: (1) the reduced nitrification efficiency in AER; and (2) the additional denitrification volume in the lower layers of the SEC. However, ASM1 & 3 (*WWTP1*) present a completely different behaviour.

There, a decrease of the S_{NHx} concentration is observed because of: (1) a lower decay rate due to its electron acceptor dependency in the mathematical representation of ASM3; and (2) a very low concentration of X_{ANO} in the upper part of the settler (see Figure 3) (ASM1 & 3). S_{NOx} also decreases (as in ASM2d) due to the additional anoxic zone in the bottom part of the SEC. Specifically, in the ASM2d implementation (*WWTP2*), the higher X_{PAO} and X_{PHA} concentrations achieved in ANAER with the reactive settler, increase the overall P uptake efficiency in both ANOX and AER zones. Hence, when a reactive settler is introduced in the plant model, there is a lower S_{PO4} concentration in the effluent (see P profile in Figure 3). Figure 4 shows the dynamic profiles of the effluent S_{NHx}, S_{NOx} and S_{PO4}. All cases have similar steady state/dynamic behaviour (Figure 2), except for S_{NHx}. In this case, the mixing/transport effect through the different layers of the settler is more important than the effect of the reactive settler i.e. S_{NHx} increases slightly.

BNR PERFORMANCE WITH REACTIVE SETTLER AND DECAY MODIFICATION (ASM1 AND 2D)

Underflow results

The soluble components (S_O, S_{NHx}, S_{NOx} and S_{PO4}) follow the same dynamics, but with different average concentrations, compared to the previous approach (see Figure 2). Nevertheless, some interesting changes can be observed in the biomass. The reduced decay rates in this third set of models increase the X_{OHO}, X_{ANO} and X_{PAO} (and consequently a reduced X_U) concentrations at the bottom of the SEC (even reaching higher concentrations than in the default case; Figure 3 shows the X_U, XC_B, X_{OHO}, X_{ANO} and X_{PAO} profiles). The influence of the high decay rates when simulating WWTPs with a reactive settler was already observed in Gernaey *et al.* (2006). Thus, in order to avoid unrealistic model predictions of ASM1 (and

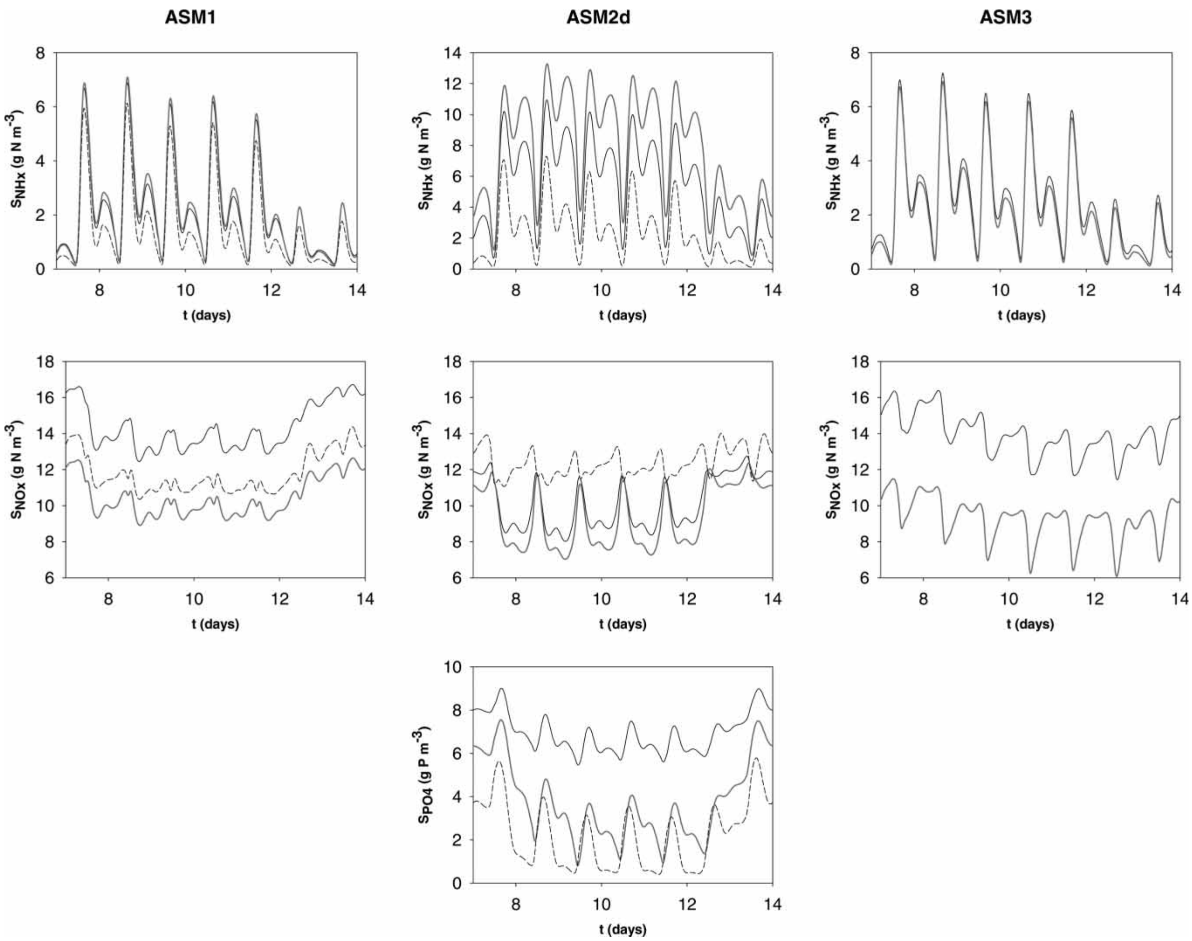

Figure 4 | S_{NHx} (first row), S_{NOx} (second row) and S_{PO4} (third row) effluent dynamic profiles for ASM1 (first column), ASM2d (second column) and ASM3 (third column). The different modelling concepts are colour coded: black (default), gray (reactive settler) and short-dashed (reactive settler + decay rate modification).

ASM2d) during low redox conditions, it was proposed to add an empirical model to take into account the S_{O2}/S_{NOx} elimination via heterotrophic growth in the secondary settler (Gernaey *et al.* 2006).

Another phenomenon to consider is the impact of the death-regeneration principle, where the decay of biomass in ASM1 and ASM2d leads to generation of new substrate (XC_B) for the heterotrophs (X_{OHO}) and P accumulating organisms (X_{PAO}). This explains the slight increase of biomass in the lower layers of the secondary settler, i.e. more hydrolysis, more growth and less decay in the ASM1 and ASM2d simulations when introducing electron acceptor dependent decay in the reactive settler model. In ASM3, the death-regeneration principle is no longer present, and thus the effect of the decay process on the biomass resulting from a reactive settler model is different. For this reason, the biomass concentration for a simulation with a reactive settler is always lower than in the default case (non-reactive settler).

Overflow results

Introduction of electron acceptor dependent decay rates in the models generally increases the overall BNR efficiency when compared to a stand-alone reactive settler implementation. S_{NHx} and S_{PO4} concentrations are lower since reduced decay under anoxic (ASM1, ASM2d) and anaerobic (ASM2d) conditions will result in increased X_{ANO} and X_{PAO} concentrations for the same sludge wastage flow rate (see Figure 3). In the ASM2d implementation, S_{NOx} increases slightly for two reasons: (1) higher nitrification efficiency, i.e. more nitrate production; and (2) improved S_F and S_{VFA} uptake by X_{PAO} leaving less available substrate for denitrification (see Figure 2). Nevertheless, in global terms, it can be said that the total S_{NOX} and total S_{PO4} are lower in the effluent as a consequence of the extra reactive volume in the secondary settler and thereby provides a better description of the biomass behaviour in the anaerobic, anoxic and aerobic biological reactors.

DISCUSSION

The results reported in this paper need a thorough discussion. An important observation is that the representation of decay rates in the original ASM1 and 2d implementations, more specifically the absence of electron acceptor dependency, makes those models less suitable to simulate BNR in *WWTP1* and *2* in case a reactive settler is used. According to experimental observations reported in Siegrist *et al.* (1999), there is a differentiation (in decay rate) amongst aerobic, anoxic and anaerobic conditions. The over-prediction of the effect of decay is especially critical in the ASM2d case, where an approximate increase in the effluent S_{NHx} of about 50% can be observed as a consequence of introducing a reactive settler with standard ASM2d reactions added to the settler model. The efficiency of the simulated N removal processes improves significantly by including a more realistic assumption that decay process rates are electron acceptor dependent.

Another important observation relates to the denitrification in the secondary settler. In the three reactive settler implementations (ASM1, 2d & 3) one can observe: (1) reduction of S_{O2} and (2) increase of the hydrolyzed XC_B, which can promote a substantial removal of S_{NOx} in the lower layers of the secondary settler (high biomass concentration). The consideration of these processes is extremely important because the whole denitrification potential of the WWTP might be underestimated if using a standard non-reactive settler model. Closely related to this phenomenon, the potential appearance of rising sludge should be mentioned. Rising sludge is characterized by appearance of rising or floating activated sludge flocs with poor settling characteristics in a relatively short period of time. The main reason for rising sludge is the conversion of nitrate to nitrogen gas. If enough gas is formed, the sludge mass becomes buoyant and rises or floats to the surface, thereby worsening the clarification efficiency. Comas *et al.* (2008) pointed out the importance of also considering microbiology related TSS separation problems during simulation studies. Rising sludge is not currently included in the available settling models, but with the reactive settler approach presented in this paper, an additional process could be included in order to also predict these (undesirable) episodes.

The S_{NOx} plays an important role during biological P removal. More specifically, the presence of S_{NOx} has a tremendous impact on the P accumulating population. A model based on a non-reactive settler overestimates the quantity of returning S_{NOx} via the external recirculation. Both X_{OHO} and X_{PAO} use the very same substrate, but the heterotrophs (X_{OHO}) have a competitive advantage due to their faster growth kinetics. This also implies that a secondary settler with high retention time could be considered as an alternative denitrification zone. Since P uptake processes in ASM2d are extremely sensitive to S_{NOx} presence, a non-reactive settler can predict unrealistic P removal efficiencies. Again, it is important to point out the importance of considering electron acceptor dependent decay rates when a reactive settler is used. Compared to aerobic conditions, lower decay rates for X_{PAO} are expected under anoxic and anaerobic conditions.

One of the main purposes of the manuscript is to provide a basis for discussion, and therefore the well-known benchmark platform was chosen for the simulations. With respect to electron acceptor dependent decay rates, the lack of such a dependency in the ASM1 and the ASM2d is a clear limitation of the predictive ability of those models. Specifically for the settler, the different cases that were simulated for the settler represent two extreme situations: on the one hand, it seems overly optimistic to assume that no reaction takes place in the settler, which corresponds to our base case (non-reactive settler), especially when there is a considerable sludge blanket at the bottom of the settler. On the other hand, it is quite clear from the presented simulation results that the predicted removal rates are too high when adopting a reactive settler model. In practice, we would expect rates to be lower in the settler, mainly because transport limitations will play a much more prominent role compared to the activated sludge tanks. In order to take into account these phenomena, diffusion coefficients could be included in the lower layers when constructing the mass balances. There is a need for experimental data from full-scale secondary settlers in order to determine how much the settler contributes to the total activity of the plant before implementing such a modification in the settler model (Henze *et al*. 1993; Chanona *et al*. 2006; Bouzas *et al*. 2007).

Finally, the importance of the WWTP model purpose or the model study objectives needs to be mentioned, since it will greatly influence the ASM selection. Assume a modelling study, where the aerobic/anoxic zones need to be refined from the results obtained by a design guideline, e.g. Metcalf & Eddy. In that case, ASM1 (only N) and 2d (combined N and P) should be used. On the other hand, if an existing facility needs to be optimized by means of mathematical modelling and a selection of control strategies or operational procedures then a combined ASM1 or ASM2d reactive settler + electron acceptor dependent decay rates or ASM3 + reactive settler would be more appropriate. Indeed, the latter ones include additional processes and it is possible to provide a plant description at a more detailed level because additional processes and interactions are considered.

This manuscript also has a warning purpose. It is indeed essential for everyone working with modelling and simulation of WWTPs to be fully aware of the dramatically different results that can be obtained due to the choice of model and model structure. The set of models investigated in this paper, i.e. ASM1, 2d and 3, reactive or non-reactive settler model, electron acceptor dependent decay rates or not, all fall within a similar category of models and still the results vary significantly. Most model users will probably not give much thought about which model structure to use and simply assume all these well-established models to produce similar results. Thereby simulation results may easily be misinterpreted and conclusions misleading, simply because users are not aware of how much the initial choice of model structure will influence the outcome of a simulation study.

CONCLUSIONS

The key findings are summarized in the following points:

1. Mathematical model structure – and as a consequence the model assumptions made when creating a WWTP model – has a strong influence on the simulated overall BNR performance;
2. Reactive settler (1) increases the hydrolysis of particulates; (2) reduces S_{NOx} concentration (bottom); (3) increases the oxidation of COD compounds and S_{NHx} (top); (4) increases X_{OHO} and X_{ANO} decay rates; and, finally (5) increases the growth of X_{PAO} and formation of $X_{PAO,Stor}$ for ASM2d;
3. The electron acceptor dependent decay modification substantially increases the concentration of X_{ANO}, X_{OHO} and X_{PAO};
4. The death-regeneration concept has a significant influence on biomass behaviour in ASM1 and ASM2d.

NOMENCLATURE

The nomenclature used in this article is in accordance with the new standardized framework for wastewater treatment modelling notation (Corominas *et al*. 2010).

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