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Computer aided model analysis and dynamic simulation of a wastewater treatment plant

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Abstract A nitrogen removal benchmark was analyzed using the Activated Sludge Models No. 1 (ASM1) and No. 3 (ASM3) in order to establish a basis for designing an experimental comparison of the two model types. Differences in steady state effluent concentrations predicted by both models could to a large extent be explained by different model concepts. The steady state system performance was analyzed by evaluating the Monod factor values, and through a sensitivity analysis of the kinetic model parameters. Both methods complement each other. Analysis of the Monod factor values can lead to determination of parameters to be estimated during model calibration. The steady state system response to manipulation of the potential actuators for control was evaluated via a sensitivity analysis. The concept of relative sensitivity was introduced to compare the relative effect of each actuator in both models. The negative relative sensitivities of X_S to four of the five control handles analyzed imply an opposite response of both models, which can be important for control structure design. The analysis of the process behavior to different disturbances showed different dynamics of both models. ASM3 simulation results are easier to interpret because the model structure is more transparent, mainly due to the simpler cell decay model principle considered in ASM3. An inverse response was obtained for the return sludge and nitrate recycle flow rate, indicating that multivariable control design is required.

List of symbols

The nomenclature followed in Gujer et al. (1999) for the ASM3 model is adopted as the base nomenclature. The notation followed in Henze et al. (1987) for the ASM1 model is given in parentheses.

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Common notation for the ASM1 and ASM3 models

k_H	Hydrolysis rate constant (k_h), g COD_{XS} (g COD_{XH})$^{-1}$ day^{-1}
K_X	Hydrolysis saturation constant (K_X), g COD_{XS} (g COD_{XH})$^{-1}$
K_{O2}	Oxygen saturation constant for X_H ($K_{O,H}$), g O_2 m^{-3}
$K_{A,O2}$	Oxygen saturation constant for X_A ($K_{O,A}$), g O_2 m^{-3}
K_{NOX}	Saturation constant for S_{NOX} (K_{NO}), g NO_3-N m^{-3}
K_S	Saturation constant for substrate S_S (K_S), g COD_{SS} m^{-3}
K_{NH4}	Saturation constant for S_{NH4} (K_{NH}), g N m^{-3}
S_{O2}	Dissolved oxygen (S_O), g O_2 m^{-3}
S_I	Inert soluble organic material (S_I), g COD m^{-3}
S_S	Readily biodegradable organic substrates (S_S), g COD m^{-3}
S_{NH4}	Ammonium plus ammonia nitrogen (S_{NH}), g N m^{-3}
S_{NOX}	Nitrate plus nitrite nitrogen (S_{NO}), g N m^{-3}
S_{ALK}	Alkalinity of the wastewater (S_{ALK}), mol m^{-3}
X_I	Inert particulate organic material (X_I), g COD m^{-3}
X_S	Slowly biodegradable substrates (X_S), g COD m^{-3}
X_H	Heterotrophic organisms ($X_{B,H}$), g COD m^{-3}
X_A	Autotrophic organisms ($X_{B,A}$), g COD m^{-3}
μ_H	Heterotrophic maximum growth rate of X_H ($\widehat{\mu}_H$), day^{-1}
μ_A	Autotrophic maximum growth rate of X_A ($\widehat{\mu}_H$), day^{-1}

Notation involved only in the ASM3 model

$b_{A,NOX}$	Anoxic endogenous respiration rate of X_A, day^{-1}
$b_{A,O2}$	Aerobic endogenous respiration rate of X_A, day^{-1}
$b_{H,O2}$	Aerobic endogenous respiration rate of X_H, day^{-1}
$b_{H,NOX}$	Anoxic endogenous respiration rate of X_H, day^{-1}
$b_{STO,O2}$	Aerobic respiration rate for X_{STO}, day^{-1}
$b_{STO,NOX}$	Anoxic respiration rate for X_{STO}, day^{-1}
$i_{SS,XI}$	SS to COD ratio for X_I, g SS (g COD_{XI})$^{-1}$
$i_{SS,XS}$	SS to COD ratio for X_S, g SS (g COD_{XS})$^{-1}$
$i_{SS,BM}$	SS to COD ratio for X_{BM}, g SS (g COD_{XBM})$^{-1}$
$i_{N,XS}$	N content in X_S, g N (g COD_{XS})$^{-1}$

$i_{N,SS}$	N content in S_S, g N (g COD_{SS})$^{-1}$
K_{ALK}	Saturation constant for alkalinity for X_H
$K_{A,NH4}$	Ammonium substrate saturation constant for X_A
$K_{A,ALK}$	Saturation constant for alkalinity for X_A, mol m^{-3}
$K_{A,NOX}$	Saturation constant for S_{NOX}, g NO_3-N m^{-3}
K_{STO}	Saturation constant for X_{STO}, g COD_{Xsto} (g COD_{XH})$^{-1}$
k_{STO}	Storage rate constant, g COD_{SS} (g COD_{XH})$^{-1}$d^{-1}
S_{N2}	Nitrogen, g N m^{-3}
X_{SS}	Suspended solids, g SS m^{-3}
X_{STO}	Cell internal storage product of heterotrophic organisms, g COD m^{-3}
η_{NOX}	Anoxic reduction factor, dimensionless

Notation involved only in the ASM1 model

b_A	Decay coefficient for autotrophic biomass, day^{-1}
b_H	Decay coefficient for heterotrophic biomass, day^{-1}
k_a	Ammonification rate, m^3 (g COD d)$^{-1}$
S_{ND}	Soluble biodegradable organic nitrogen, g N m^{-3}
X_{ND}	Particulate biodegradable organic nitrogen, g N m^{-3}
X_P	Particulate products arising from biomass decay, g COD m^{-3}
η_h	Correction factor for hydrolysis under anoxic conditions, dimensionless
η_g	Correction factor for growth under anoxic conditions, dimensionless

General symbols and abbreviations

ASM1	Activated Sludge Model No. 1
ASM3	Activated Sludge Model No. 3
C	Carbon
COST	European Cooperation in the field of Scientific and Technical Research
ICAS	Integrated computer aided system
K_La	Oxygen transfer coefficient, day^{-1}
MoT	Model test bed tool of ICAS
N	Nitrogen
P	Phosphorus
PCA	Principal component analysis
p_j	Parameter j
R_i	Reactor i (1 to 5)
S_{ij}	Sensitivity of the model component i to parameter p_j
y_i	Model output (prediction) for the component j
Δ	Increment
ψ_{pj}	Scaling factor for the parameter p_j

Introduction

Activated sludge processes are among the most widespread biological wastewater treatment techniques. Here a bacterial biomass suspension is responsible for the removal of pollutants. Besides removal of organic carbon (C) substances, an activated sludge wastewater treatment plant can achieve biological nitrogen (N) removal and biological phosphorus (P) removal, depending on its design and operation and on the composition of the inlet wastewater.

Increased knowledge about the biological degradation mechanisms in the activated sludge has resulted in a number of mathematical models (e.g. Henze et al. 1987, 1995; Gujer et al. 1999; Barker and Dold 1997a, 1997b) that have been applied for understanding the process behavior and for scenario evaluations. Modeling and simulation are indeed important tools for generation and assessment of scenarios related to wastewater treatment plant design and operation. For wastewater treatment, a clean process can be understood as producing an effluent that is in compliance with the effluent standards. Modeling and simulation allow the investigation of the feasibility and potential benefits of various control strategies that may be implemented, with the aim to stabilize the operation of the actual plant and further to ensure high performance even when large disturbances are experienced.

The disturbances are indeed a key issue in wastewater treatment plant design and operation. The plants should ideally be able to handle significant load variations. The diurnal and weekly variations under dry weather conditions include two- to threefold flow rate variations. Under heavy rain and storm conditions the maximal flow rate can be up to five times higher than that under dry weather conditions. The traditional design approach for these cleaning plants is to apply a significant over-design under dry weather conditions, often with very little control. However, even these over-designed plants are often not able to handle either heavy rains or storm weather conditions without spillage of part of the untreated wastewater. These unsatisfactory design and control issues call for a closer analysis using computer aided process engineering tools. Thus, the purpose of this paper is to demonstrate how a plant-wide computer aided model analysis and dynamic simulation tool may be used to evaluate the modeled plant behavior. Two activated sludge models are compared, ASM1 and ASM3. The ASM1 model (Henze et al. 1987) has become a major reference for many scientific and practical projects and has been implemented (in some cases with modifications) in most of the commercial software available for modeling and simulation of wastewater treatment plants for N removal. However, during its usage and application some defects of this model have become apparent (Gujer et al. 1999). The ASM3 model (Gujer et al. 1999) is intended to provide better description of the microbiological processes taking place in a wastewater treatment plant for biological N removal. Therefore this paper provides an exhaustive comparative analysis of the two activated sludge models on a benchmark case to provide a basis for experimental comparison of the two models for the purpose of implementation of control strategies on an N removal treatment plant.

The evaluation is based upon static model analysis and dynamic simulation of the effect of idealized disturbances and control actions. The idealized conditions considered are an average static dry weather wastewater load scenario superimposed with pulse disturbances for dynamic simulation. These idealized conditions are selected to elucidate differences between the two models around average dry weather conditions.

The structure of the paper is as follows. First, a generic continuous nitrogen removal plant is introduced. Activated Sludge Model No. 1 (ASM1) and Activated Sludge Model No. 3 (ASM3) are presented, highlighting their main differences. Analysis and comparison of the performance of the two models upon the generic nitrogen removal plant are performed. Subsequently, sensitivity analysis results of both models on model parameters and potential actuators for control are compared. Finally, the dynamic response of both models to pulse and step disturbances on influent load and control handles are studied.

Methods

Nitrogen removal plant

Some common plant configurations for implementing biological N removal on a wastewater treatment plant are the predenitrification plants, oxidation ditch plants, alternating plants, sequencing batch reactors, etc. Process design and operation design to achieve optimal treatment plant operation might be very different depending on the actual treatment plant configuration. Model-based scenario evaluation is therefore an important tool to select appropriate process and control structures resulting in minimum wastewater treatment cost.

In this paper the COST benchmark wastewater treatment plant is used as an illustrative example (Fig. 1). A full description of the plant can be found in Copp (2002). The treatment plant is a predenitrification system consisting of two anoxic reactors, three aerated reactors and a secondary settler. The system includes two recycle streams, one from the last aerated reactor to the first anoxic reactor, and a second one, which is sludge recycle, from the secondary settler to the first anoxic reactor. In the aerated tanks, N components are oxidized to obtain nitrate nitrogen. The first recycle stream (internal recycle) is used to pump the nitrate rich (nitrified) mixed liquor back to the anoxic zone. In the anoxic zone denitrification (reduction of nitrate to nitrogen gas using a carbon source as electron donor) takes place. The second recycle stream (sludge recycle) is used to pump the thickened activated sludge from the bottom of the secondary settler to the first anoxic tank, where it is mixed with the incoming wastewater. This system cannot achieve 100% nitrogen removal because the last aerobic zone discharges a fraction of the nitrified mixed liquor into the secondary settler. Thus, to be efficient these systems require a relatively high internal recycle to feed flow rate ratio. At the nominal operating point this ratio is 3.0 corresponding to a mean fluid phase residence time (based on total volume) of 15.6 h, and the sludge recycle flow rate ratio is 1.0 corresponding to a mean sludge residence time (sludge age) of approximately 9.1 days.

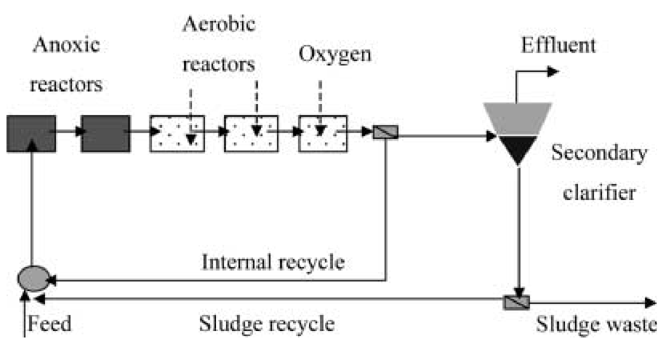

Fig. 1. Plant configuration used for the case study

Mathematical models

Biological N removal process modeling has mainly relied on the ASM1 model (Henze et al. 1987). As such, ASM1 has evolved into a standard model for evaluation of control strategies to improve operation of biological nitrogen removal wastewater treatment plants. The most illustrative example of this usage of the ASM1 model is probably the COST (European Cooperation in the field of Scientific and Technical Research) benchmark wastewater treatment plant (Copp 2002). The ASM1 model has, however, proven difficult to calibrate to real plant data (Petersen et al. 2002a).

Recently, Gujer et al. (1999) proposed the ASM3 model as an alternative to the ASM1 model for modeling of biological N removal processes. The ASM3 model should become a standard model, and corrects for defects that have appeared during the usage of the ASM1 model.

The major difference between the ASM1 and ASM3 models – illustrated in Fig. 2 – is that the latter recognizes the importance of storage polymers in the heterotrophic conversions in the activated sludge processes. In the ASM3 model, it is assumed that all readily biodegradable substrate (S_S) is first taken up and stored in an internal cell component (X_{STO}) prior to growth (see Fig. 2). The biomass is thus modeled with an internal cell structure. The internal component X_{STO} is subsequently used for biomass growth in the ASM3 model. Biomass growth directly on external substrate as described in ASM1 is not considered in ASM3. Furthermore, the death regeneration concept of ASM1 is replaced in ASM3 by endogenous respiration, which is believed to be closer to the phenomena observed in reality. As a result, the conversion processes of both groups of organisms (autotrophs and heterotrophs) are clearly separated in ASM3, whereas the decay regeneration cycles of the autotrophs and heterotrophs are strongly interrelated in ASM1 (see Fig. 2). Finally, ASM3 allows a differentiation between aerobic and anoxic biomass decay whereas ASM1 does not (not shown in Fig. 2).

Modeling and simulation aspects

Two dynamic mathematical models of the nitrogen removal plant have been implemented based on the ASM1 and ASM3 models. The secondary settler was modeled using the double-exponential settling velocity function of Takacs et al. (1991).

To facilitate the analysis, a set of scaling factors (ψ) is introduced into the process rate expressions of the ASM1 and ASM3 models; i.e. the reference value of the model parameters (p) and control handles to be analyzed are affected by the corresponding scaling factor (ψ_p). This allows , for instance, parametric sensitivity and model analysis to be performed through variation of the scaling factors.

A few illustrative model equations of the ASM1 and ASM3 models including the scaling factors ψ_p are presented below:

The hydrolysis process rate expression for the ASM1 model is:

$$r_{h_{\mathrm{ASM1}}} = \psi_{k_h} k_h \left(\frac{\frac{X_S}{X_H}}{\psi_{K_X} K_X + \frac{X_S}{X_H}} \right) \times \left[\left(\frac{S_{O2}}{\psi_{K_{O2}} K_{O2} + S_{O2}} \right) + \psi_{\eta_h} \eta_h \left(\frac{\psi_{K_{O2}} K_{O2}}{\psi_{K_{O2}} K_{O2} + S_{O2}} \right) \left(\frac{S_{NOX}}{\psi_{K_{NOX}} K_{NOX} + S_{NOX}} \right) \right] X_H \quad (1)$$

However, for the ASM3 model the hydrolysis process rate expression is:

$$r_{h_{\mathrm{ASM3}}} = \psi_{k_h} k_h \left(\frac{\frac{X_S}{X_H}}{\psi_{K_X} K_X + \frac{X_S}{X_H}} \right) X_H \quad (2)$$

Model implementation and tools

The dynamic wastewater treatment plant models were implemented and solved using the Integrated Computer-Aided System (ICAS) (Gani et al. 1997). ICAS combines computational toolboxes for modeling, simulation, synthesis/design, control and analysis in a single integrated system. To model complete wastewater treatment plants, process units were modeled as individual modules and incorporated into the ICAS model library improving model reusability. Specifically, the models are written, tested and exported to the ICAS model library using the Model Test bed tool (MoT). MoT is an equation based modeling tool to analyze, solve and optimize a model. Once the user-defined models are available from the ICAS model library, they can be used to set up the plant flow sheet in the ICAS environment and to apply the other ICAS toolboxes, such as the control toolbox.

Backward Difference Formulae and Implicit Euler methods with error control were used to solve the dynamic plant models. Both methods are available from the ICAS solver library.

Results and discussion

Simulation problem definition

In this work, a predenitrification plant for nitrogen removal (Fig. 1) case study is simulated based on the ASM1 and ASM3 models. Steady state conditions for a given set of constant wastewater specifications and reference parameter values are reached by performing dynamic simulation runs. The simulations are repeated with perturbed parameter values. The simulation results are used to perform steady state sensitivity analysis on model parameters and potential control handles, to evaluate the system performance, and to detect differences between the behaviors obtained with the two models.

Wastewater specifications

In order to correctly compare and analyze simulated results based on the ASM1 and ASM3 models for this case study, compatible sets of specifications for the incoming wastewater stream are defined for both models. The average values corresponding to the dry weather scenario from the COST benchmark study are considered as the ASM1 wastewater specifications (Copp 2002). The wastewater component concentrations for the ASM3 model were adopted to obtain exactly the same C and N load for both models. Table 1 summarizes the influent component concentrations used for both models. For ASM3, the reference stoichiometric factors for N given by Gujer et al. (1999) were used, except $i_{N,XS}$. The stoichiometric factor $i_{N,XS}$, representing the fraction of N in slowly biodegradable substrate in ASM3, was slightly adjusted (from 0.04 to 0.0426) in order to keep the same concentration of N included in particulate matter for both models.

Model parameters

In this work, the stoichiometric and kinetic constants at 15 °C included in the COST benchmark study report (Copp 2002) were used for the ASM1 model. For the ASM3 model the parameter values were interpolated to 15 °C based on the default parameter values at 10 and 20 °C and the temperature interpolation function given by Gujer et al.

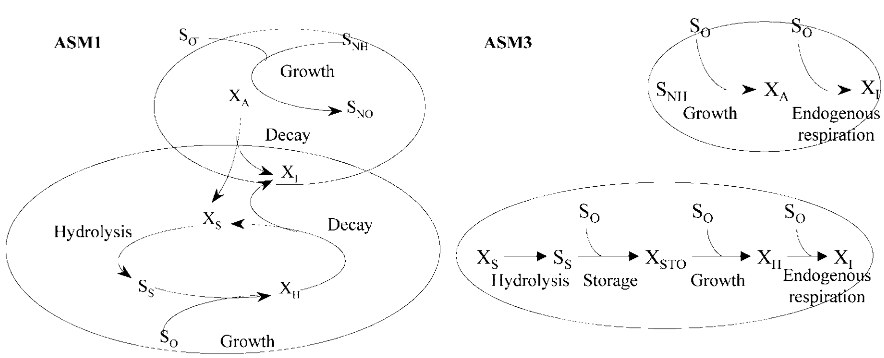

Fig. 2. Substrate flows in the ASM1 and ASM3 models (modified from Gujer et al. 1999)

(1999). The stoichiometric factor $i_{N,XS}$ of the ASM3 model was slightly modified as explained above.

Steady state simulation results

The above-mentioned constant influent wastewater specifications and model parameter values were used to obtain the corresponding steady state values for both models. A 100-day simulation time horizon was adopted to ensure that steady state is reached. Table 2 lists the component concentration values reached with both models at steady state for reactors R1 and R5 as examples.

The particulate inert compounds (X_I) are not involved in any conversion process in the ASM1 model. In the ASM3 model, the anoxic and aerobic decay processes of heterotrophic (X_H) and autotrophic (X_A) biomass release particulate inert components. This fact partly explains the difference between X_I predictions resulting from both models. In the ASM1 model inert material arising from biomass decay processes is represented by X_P. Steady state simulation results in Table 2 indeed show that the sum of the concentration of particulate products resulting from biomass decay (X_P) and the concentration of inert material (X_I) for ASM1 is relatively close to the steady state X_I concentration predicted with the ASM3 model.

The heterotrophic organisms grow on a storage compound substrate (X_{STO}) in the ASM3 model, whereas in ASM1 they consume the readily degradable substrate (S_S) directly. Thus, the remaining high concentration of X_{STO} (available for growth) in the ASM3 model can partly explain the large difference in the heterotrophic biomass (X_H) concentration between the two models at steady state. Another factor that causes the difference in the X_H concentrations between the two models is the large differences in the steady state concentrations of the slowly biodegradable substrate (X_S) predicted by ASM1 and ASM3. As described in Fig. 2, the ASM1 model considers the death regeneration concept whereas the ASM3 model adopts the endogenous respiration concept to describe biomass decay. These different assumptions imply that the slowly biodegradable substrate (X_S) is involved in two clearly different ways in both models. For ASM3, X_S is present in the incoming wastewater and is converted by hydrolysis. For ASM1, X_S is also consumed via hydrolysis. However, it is simultaneously produced due to biomass decay according to the ASM1 death regeneration concept. Clearly, the hydrolysis process rates are much higher in ASM1 compared to ASM3. The lower steady state concentration of X_S in ASM1, in comparison with ASM3, indicates that more X_S has been converted to biomass (X_H) in ASM1 (see also Fig. 2 for substrate cycles), and can thus explain part of the X_H concentration differences predicted by both models.

The effluent S_{NH4} concentrations predicted by ASM3 are significantly higher compared to ASM1. Clearly, both models result in a different distribution of the N components when standard kinetic parameters are used. Here, care was taken in defining an ASM3 influent composition such that both model evaluations (ASM1 and ASM3) are carried out for identical N and COD loads. The ASM3 effluent S_{NH4} concentration could be closer to the value predicted by the ASM1 model by changing the ASM3 model parameters that are related to nitrification. However, model calibration is not a first priority in this paper, and it was preferred to use the standard set of parameters for the ASM3 model since that has also been done for the ASM1 based model (Copp 2002).

Analysis of Monod factors

In the activated sludge systems, most processes are closely interlinked and involve a number of substrates, intermediates and degradation products. The reaction rates are most often described by Monod-type kinetics. As a first step of the model analysis, the actual values of the Monod factors can be used as an indication pointing to the substrates limiting the process rates. Table 3 lists the actual values of the Monod factors for the ASM1 and ASM3 models at steady state conditions (after a 100-day simulation run, as mentioned above).

Table 1. Wastewater specifications for the ASM1 and ASM3 models

Components	ASM1-COST	ASM3
S_I	30.00	30.00
S_S	69.50	69.50
X_I	51.20	51.20
X_S	202.32	202.32
X_H	28.17	28.17
X_A	0	0
X_P	0	–
S_{O2}	0	0
S_{NOX}	0	0
S_{NH4}	31.56	36.43[a]
S_{ND}	6.95	–
X_{ND}	10.59	–
S_{ALK}	7.00	7.00
X_{SS}	–	215.49[b]
S_{N2}	–	0
X_{STO}	–	0

[a] $S_{NH4\text{-}ASM3}=S_{NH4\text{-}ASM1}+(S_{ND\text{-}ASM1COST}-i_{N,SS}S_{S\ ASM1COST})$
[b] $X_{SS}=i_{SS,XI}X_I+i_{SS,XS}X_S+i_{SS,BM}(X_A+X_H)+i_{SS,XSTO}X_{STO}$
$i_{N,XS}$=0.0426 (in contrast to the ASM3 default value: 0.04)

Table 2. Simulated steady state values in reactors R1 and R5 for ASM1 and ASM3 respectively (model component concentrations)

Variable	R1		R5	
	ASM1	ASM3	ASM1	ASM3
S_I	30	30	30	30
S_S	2.81	2.01	0.889	0.245
X_I	1149.	1423.9	1149.	1426.1
X_S	82.1	293.7	49.3	262.2
X_H	2552.	1751.2	2559	1759.9
X_A	148.	144.9	150.	146.3
X_P	449.	–	452.	–
S_O	0.00430	0.00273	0.491	0.276
S_{NOX}	5.37	5.62	10.4	10.1
S_{NH4}	7.92	11.52	1.73	4.63
S_{ND}	1.22	–	0.688	–
X_{ND}	5.28	–	3.53	–
S_{ALK}	4.93	4.71	4.13	3.87
X_{SS}	–	3223.9	–	3207.1
S_{N2}	–	24.6	–	27.7
X_{STO}	–	382.1	–	375.5

Table 3. Actual values of Monod factors for the ASM1 and ASM3 models. R1 to R5 represent the different reactors in the plant configuration studied (see Fig. 1)

Factor	R1		R2		R3		R4		R5	
	ASM1	ASM3	ASM1	ASM3	ASM1	ASM3	ASM1	ASM3	ASM1	ASM3
$\frac{S_S}{\psi_{K_S} K_S+S_S}$	0.210	0.501	0.127	0.223	0.103	0.104	0.090	0.096	0.081	0.109
$\frac{S_{O2}}{\psi_{K_{O2}} K_{O2}+S_{O2}}$	0.021	0.014	0.000	0.000	0.895	0.879	0.923	0.900	0.710	0.579
$\frac{S_{O2}}{\psi_{K_{A_{O2}}} K_{A_{O2}}+S_{O2}}$	0.010	0.005	0.000	0.000	0.811	0.745	0.858	0.783	0.551	0.355
$\frac{S_{NOX}}{\psi_{K_{NOX}} K_{NOX}+S_{NOX}}$	0.914	0.918	0.879	0.885	0.928	0.930	0.948	0.950	0.954	0.952
$\frac{S_{NOX}}{\psi_{K_A NOX} K_A NOX+S_{NOX}}$	–	0.918	–	0.885	–	0.930	–	0.950	–	0.953
$\frac{S_{NH4}}{\psi_{K_{NH4}} K_{NH4}+S_{NH4}}$	0.887	0.999	0.893	0.999	0.847	0.998	0.748	0.998	0.633	0.997
$\frac{S_{NH4}}{\psi_{K_A NH4} K_A NH4+S_{NH4}}$	–	0.920	–	0.921	–	0.897	–	0.853	–	0.822
$\frac{X_{STO}/X_H}{\psi_{K_{STO}} K_{STO}+X_{STO}/X_H}$	–	0.179	–	0.180	–	0.178	–	0.177	–	0.176
$\frac{S_{ALK}}{\psi_{K_{ALK}} K_{ALK}+S_{ALK}}$	–	0.979	–	0.980	–	0.978	–	0.976	–	0.975

For both models, the Monod factor values related to oxygen (S_{O2}), nitrate (S_{NOX}) and ammonium (S_{NH4}) show relatively high values for the aerobic reactors (R3, R4 and R5) for both autotrophic (rows 3, 5 and 7) and heterotrophic growth (rows 2, 4 and 6). It is only in the last aerobic reactor that S_{O2} seems to be more rate limiting. This fact can be explained by the lower oxygen transfer coefficient (K_La) in this reactor (84 day^{-1} for R5 versus 240 day^{-1} for R3 and R4). Contrarily, a low value is observed for the readily biodegradable substrate (S_S). For ASM1, this suggests that heterotrophic growth in the aerobic reactors is limited mainly by this component, and that the Monod saturation constant for S_S (K_S) plays an important role in the simulations. For ASM3, on the other hand, uptake of S_S in the aerobic zones is limited by the S_S concentrations, whereas heterotrophic growth on the cell-internal storage component (X_{STO}) is limited by the X_{STO} concentration in all reactors.

The Monod factor values for the anoxic reactors (R1 and R2) show again that S_S is the limiting substrate for both models.

Specifically for the ASM3 model, the effect of S_{NH4} limitation on the heterotrophic growth process can be ignored, whereas S_{NH4} has a slight effect on the autotrophic biomass growth rate. The effect of alkalinity (S_{ALK}) is also negligible.

By simply using these Monod factor values a quick indication of the critical processes that limit the process rates and, consequently, the system performance, is provided. Based on this analysis, it can be concluded that denitrification in the anoxic zones could be improved by adding more readily biodegradable substrate (S_S) into the anoxic reactors, whereas nitrification could be improved by increasing the aeration capacity (K_La) in R5. Below, a more rigorous and general sensitivity analysis will be presented. It is important to note that the results obtained from both methods (evaluation of Monod factor values and sensitivity analysis) are case-specific. This means that the analysis results are applicable for the specific treatment plant configuration shown in this paper, whereas the conclusions may be completely different for different operating conditions and plant configurations.

Sensitivity analysis

A steady state sensitivity analysis of the model predictions to both model parameters and potential control handles is presented for the ASM1 and ASM3 models. Equation (3) defines the sensitivity S_{ij} as the ratio of the relative change of the model prediction y_i to the relative change of a given parameter p_j (van Veldhuizen et al. 1999; Meijer et al. 2001; Petersen et al. 2002b):

$$S = \frac{\frac{\Delta y_i}{y_i}}{\frac{\Delta p_j}{p_j}} = \frac{\frac{\Delta y_i}{y_i}}{\psi_{pj} - 1} \qquad (3)$$

where ψ_{pj} is the scaling factor for the parameter p_j.

The model sensitivity analysis on the model parameters and potential control handles, using a constant influent composition as previously described, was carried out by changing the value of a given parameter +0.01% with respect to its reference value. To ensure that steady state conditions are reached, a 100-day simulation time horizon (or about five sludge ages) was again adopted with constant average inlet conditions. The simulated steady state values for each perturbed parameter were compared to the reference simulation. The ASM1 and ASM3 reference simulations refer to the simulation runs including the above-mentioned reference parameter values, and the corresponding steady state results (Table 2).

The sensitivity analysis results are presented in a graphical form by using arbitrary sensitivity ranges to condense all the information into a compact representation. Sensitivities lower and higher than two predefined values are uncolored and black-colored, respectively. The corresponding sign indicates a positive or negative sensitivity value. A gray scale is used to define the different sensitivity ranges between the extreme values.

Table 4. ASM1 model sensitivity analysis to the model parameters

Comp	k_H					k_a					K_{NH4}					K_{NOX}					$K_{A,O2}$					K_{O2}					K_X				
	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5
S_{ALK}	+	+	+	+	+	0	0	0	0	-	+	+	+	+	+	0	0	-	-	-	+	+	+	+	+	+	+	0	+	+	0	-	-	-	-
S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S_{ND}	0	+	+	-	-	-	-	-	-	-	0	-	+	+	0	0	-	+	+	+	0	-	+	0	0	0	-	0	0	0	0	-	-	+	+
S_{NH4}	-	-	-	-	-	+	+	+	+	+	+	+	+	[illegible]	+	+	+	+	+	+	+	+	+	[illegible]	+	-	-	-	-	-	+	+	+	+	+
S_{NOx}	-	-	-	-	-	+	+	+	+	0	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+
S_{O2}	+	+	-	+	+	-	-	0	0	-	-	+	+	+	-	-	-	0	0	-	+	-	+	+	+	-	+	+	+	+	-	-	+	-	-
S_S	+	+	0	-	-	0	0	0	0	0	+	+	0	+	+	+	+	0	+	+	+	0	0	+	+	+	+	0	+	+	-	-	-	+	+
X_A	0	0	0	0	0	0	0	0	0	0	-	-	-	-	-	0	0	0	0	0	-	-	-	-	-	0	0	0	0	0	0	0	0	0	0
X_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	-	0
X_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X_{ND}	-	-	-	-	-	0	0	0	0	0	+	+	0	0	+	+	+	+	+	+	0	0	0	0	+	+	+	+	+	+	+	+	-	+	+
X_P	0	+	+	+	0	0	0	0	0	0	-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	0	0	0	0
X_S	-	-	-	-	-	0	0	0	-	0	+	+	+	0	0	+	+	+	+	+	+	+	+	0	0	+	+	+	+	+	+	+	-	+	+

Comp	K_S					η_g					μ_A					μ_H					η_h					b_A					b_H				
	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5	R1	R2	R3	R4	R5
S_{ALK}	0	0	-	0	-	+	+	+	+	+	-	-	-	-	-	+	0	0	0	0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S_{ND}	0	+	+	0	0	0	-	0	0	+	0	+	-	-	-	0	0	0	0	0	+	+	-	-	-	0	-	+	+	0	+	+	[illegible]	[illegible]	[illegible]
S_{NH4}	+	0	+	0	+	-	-	-	-	-	-	-	-	-	-	-	-	0	0	0	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+
S_{NOx}	+	+	+	+	0	-	-	-	-	-	+	+	+	+	[illegible]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
S_{O2}	+	+	0	0	-	+	+	+	+	+	+	+	-	-	+	-	0	0	0	0	+	-	+	+	+	-	-	+	+	-	-	-	-	-	[illegible]
S_S	[illegible]	+	+	[illegible]	[illegible]	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	+	+	-	-	-	+	+	0	+	+	+	+	+	+	+
X_A	0	0	0	0	0	0	0	0	0	0	+	+	+	+	+	0	0	0	0	0	0	0	0	0	0	-	-	-	-	-	0	0	0	0	0
X_H	0	0	-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	-	-	-	-
X_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X_{ND}	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-	0	0	0	0	+	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+
X_P	-	0	0	0	0	0	0	0	0	0	0	+	0	+	0	0	+	0	+	0	0	+	0	+	0	0	+	+	+	0	+	+	+	+	+
X_S	0	-	0	-	-	+	+	+	+	0	-	-	-	-	-	0	0	+	0	0	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+

Sensitivity Ranges: <0.1; 0.1-0.5; 0.5-1.5; 1.5-3.0; >3.0

Table 5. ASM3 model sensitivity analysis to the model parameters

Comp.	K_S					K_{NH4}					K_{ALK}					μ_A					K_X					k_H					k_{STO}					K_{STO}					μ_H					$b_{A,O2}$					$K_{A,NOx}$				
	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
S_{ALK}	-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	-	-	[illegible]	[illegible]	-	-	-	-	-	+	+	+	+	+	0	0	+	0	0	-	0	0	-	-	0	+	+	+	+	+	+	+	+	+	-	0	0	0	0
S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S_{N2}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+	0	+	0	0	0	-	0	-	-	-	+	+	+	+	+	-	-	-	-	-	0	0	0	0	0
S_{NH4}	0	0	+	0	0	0	0	0	0	0	0	0	0	0	0	-	-	-	-	-	-	-	-	-	-	0	0	+	+	+	0	0	0	-	-	0	0	+	+	+	-	0	-	-	-	+	+	+	+	+	-	0	-	-	-
S_{NOx}	+	+	+	+	0	0	0	0	0	0	0	0	0	0	0	+	+	+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	0
S_{O2}	0	+	0	0	0	0	0	0	0	0	0	0	0	0	0	-	-	-	-	[illegible]	+	+	+	+	+	-	-	0	-	-	-	0	+	0	0	0	+	+	0	0	-	-	0	0	0	+	+	+	+	+	-	0	0	0	-
S_S	[illegible]	+	+	[illegible]	[illegible]	0	0	0	0	0	0	0	0	0	0	-	-	+	+	+	-	-	-	0	0	0	+	+	0	-	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-	+	+	0	-	-	0	0	0	0	0
X_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	+	[illegible]	[illegible]	[illegible]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	+	0	0	0	0	0	0	-	-	-	-	-	0	0	+	+	0
X_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	0	0	0	-	-	0	-	0	-	0	+	+	+	0	0	0	0	0	0	-	-	-	-	-	+	+	+	+	+	0	0	0	0	0	0	0	0	0	0
X_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	0	0	0	0	0	0	-	0	0	0	+	0	+	0	+	0	0	0	0	+	0	0	0	0	0
X_S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	0	0	+	+	+	+	+	-	-	-	-	-	0	0	0	0	0	0	+	+	0	+	-	0	0	-	0	0	0	0	0	0	0	0	0	0	0
X_{SS}	0	0	0	-	0	0	0	0	0	0	0	0	0	0	0	+	+	+	0	+	+	+	+	+	+	-	-	-	-	-	0	0	0	0	0	0	0	0	-	0	0	0	0	0	0	0	0	0	-	0	0	0	0	0	0
X_{STO}	0	-	0	0	0	0	0	0	0	0	+	0	+	+	+	0	-	0	0	0	-	-	-	-	-	+	+	+	+	+	+	0	0	0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-	-	-	-	-	0	0	0	+	0	0	0	0	0	0

Comp	$b_{A,NOx}$					$b_{H,NOx}$					$b_{H,O2}$					$b_{STO,NOx}$					$b_{STO,O2}$					η_{NOX}					$K_{A,NH4}$					$K_{A,O2}$					K_{NOx}					K_{O2}					$K_{A,ALK}$				
	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
S_{ALK}	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0	+	+	0	0	0	+	+	0	0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	-	0	0	0	-	-	0	0	0	-	+	+	+	+	+
S_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S_{N2}	-	0	-	-	-	+	+	+	+	+	0	0	+	+	-	+	+	+	0	+	0	0	-	-	-	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	-	0	-	-	-	+	+	+	+	+	-	0	-	-	-
S_{NH4}	+	+	+	+	+	-	0	-	-	-	+	+	-	-	+	-	0	-	-	-	0	0	+	+	+	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+	0	0	+	+	+	-	-	-	-	-	+	+	+	+	+
S_{NOx}	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0	0	0	-	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	+	+	+	+	0	-	-	-	-	-	-	-	-	-	-
S_{O2}	+	+	+	+	+	0	0	0	0	0	-	-	0	0	-	0	+	0	0	0	-	-	0	-	-	+	+	+	+	+	+	+	+	+	+	[illegible]	+	+	+	+	-	-	0	0	-	[illegible]	+	+	+	+	+	+	+	+	+
S_S	0	+	0	0	-	+	+	+	+	+	+	+	+	+	+	0	+	+	0	0	+	+	+	+	+	-	-	-	-	-	0	+	0	0	-	0	+	0	0	-	+	+	0	0	0	0	+	+	0	+	0	+	0	0	-
X_A	-	-	-	-	-	+	0	+	+	+	0	-	+	+	0	0	0	0	0	0	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-
X_H	0	0	0	0	0	-	-	-	-	-	-	-	-	-	-	-	0	0	0	-	-	0	-	0	-	0	+	0	+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	0	0	0	0	+	0	0	0	0	0	0
X_I	0	0	0	0	+	+	0	+	0	+	+	+	+	0	+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	+	0	0	0	0	0	0	0	0	0	+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X_S	0	0	0	0	0	0	+	+	0	+	+	+	+	0	+	0	0	+	0	0	0	0	+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X_{SS}	0	0	0	-	0	-	-	-	-	-	-	-	-	-	-	0	0	0	-	0	0	0	-	-	0	0	0	0	-	0	0	0	0	-	0	0	0	0	-	0	+	0	0	0	+	+	+	0	0	+	0	0	0	-	0
X_{STO}	0	0	0	+	0	+	+	+	+	+	+	+	+	+	+	0	-	0	0	0	-	-	-	-	-	-	-	-	-	-	0	0	0	0	0	0	-	0	0	0	+	+	+	+	+	+	+	+	+	+	0	0	0	0	0

Sensitivity ranges: <0.1; 0.1-0.5; 0.5-1.5; 1.5-3.0; >3.0

Model sensitivity to model parameters

The results of the ASM1 and ASM3 model sensitivity analysis to model parameters are presented in Tables 4 and 5, respectively. In this study, only the kinetic constants of the process rate expressions were considered, and no analysis of the stoichiometric parameters is included. The main sensitivity analysis results for both models are highlighted below.

ASM1 model For the ASM1 model (Table 4), the decay coefficient for heterotrophic biomass (b_H) shows high sensitivity values on most of the model components. Indeed, nine of the 13 model components in reactor R5 show sensitivity values in the range 0.48–1.1. This is because the heterotrophic organisms use COD in a cyclic reaction scheme in the ASM1 model according to the death–regeneration principle: biomass decay feeds slowly biodegradable substrates (X_S) into hydrolysis, and triggers additional biomass growth, which consumes additional S_{O2} (Fig. 2). This cycle explains the negative sensitivity values of the S_{O2} and X_H components, and the positive value of the S_S component. The positive value for S_{NH4} (ammonium) is explained by additional hydrolysis of organic nitrogen arising from the decay of heterotrophs. The negative sensitivity value observed for S_{NOX} with respect to b_H can be explained by a net improvement in the denitrification process due to an increase in the available amount of S_S in the anoxic zone.

The Monod saturation constant for S_{NH4} (K_{NH4}) has an increasing impact on the nitrification process – in the aerobic zone – as the treatment progresses; i.e. a higher effect as the liquid flows from reactor R3 to R5. This trend was also reflected by the Monod factor values (Table 3). As nitrification proceeds along the aerobic reactors, the S_{NH4} concentration becomes lower and K_{NH4} becomes more influential on the process rate.

The Monod saturation constant for S_{NOX} (K_{NOX}) has a minor effect on the model component concentrations. The highest sensitivity value (0.19) corresponds to the S_{NOX} concentration in R2, where the corresponding Monod factor value (0.88) was lower and thus more influential on the process rate.

As the oxygen concentration in the anoxic zone has to be as low as possible, it is reasonable that the model sensitivity with respect to the oxygen Monod saturation constant for heterotrophic biomass (K_{O2}) shows a high value for the S_{O2} concentration in the anoxic zone. A higher sensitivity of S_{O2} in the last aerobic reactor compared to the first two aerobic ones is due to the lower K_La value for this reactor (compared to the other aerobic units), resulting in a lower S_{O2} concentration in this reactor.

The largest sensitivity values with respect to the oxygen saturation constant for autotrophic biomass ($K_{A,O2}$) are observed for S_{NH4} in the aerobic zone, indicating that the nitrification process rate is limited by the low S_{O2} concentration. The negative sensitivity values in the aerobic zone for X_A and S_{NOX}, and positive values for S_{NH4} and S_{O2} components indeed point towards a deterioration of the nitrification process at increased $K_{A,O2}$ values.

As expected, the S_S concentration is sensitive to the Monod saturation constant K_S because of its low concentration in the liquid phase, as also indicated by the analysis of the Monod factor values (see Table 3).

The hydrolysis rate constant k_H and the hydrolysis saturation constant K_X influence X_S and X_{ND} concentrations to the same extent (but in opposite direction) in all the reactors. This trend is also observed by perturbing other model parameters, such as b_H and η_h, but k_H and K_X show the highest sensitivity values.

The correction factor for hydrolysis under anoxic conditions (η_h) exerts the strongest influence on the S_{NOX} concentration in the anoxic zone. An increase of the hydrolysis will indeed cause an increased S_S production and, thus, an increased denitrification (consumption of S_{NOX}) in the anoxic zone. As expected, the effect of a change on η_h is less important in the aerobic reactors, and the sensitivity values of X_{ND} and X_S become comparable to the S_{NOX} sensitivity.

ASM3 model For the ASM3 model sensitivity to model parameters, only the sensitivity of S_S is very significant with respect to the saturation constant K_S (Table 5). This fact is not completely surprising (see also Table 3), because the parameter K_S is involved in the process rate equations that describe the S_S removal rate. Similarly, a change on the hydrolysis rate constant k_H will strongly influence the X_S concentration, X_S being the substrate for the hydrolysis reaction.

It can be observed that the saturation constant for S_{NH4} (K_{NH4}) has no influence on the predicted component concentrations for the numerical accuracy used in this study. The wastewater influent specifications used determine a high steady state concentration of S_{NH4} in the system, resulting in a Monod factor for this constant of almost 1 (>0.997 for all the reactors, see Table 3). Thus, results from both analyses point in the same direction.

Only the storage component concentration (X_{STO}) is sensitive to the alkalinity saturation constant for X_H (K_{ALK}), but the sensitivity value is quite low (between 0.026 and 0.027 for all the reacting units). It can be stated that K_{ALK} has no real influence on the simulation results.

The above results can be used to propose model simplifications, where model parameters have a negligible influence on the predicted concentrations.

The highest ASM3 model sensitivities are those corresponding to the model components involved in the nitrification process (S_{NOX}, S_{NH4}, S_{O2}, and to a lesser extent X_A) when the maximum specific growth rate of autotrophic biomass (μ_A) is perturbed (e.g. the S_{NH4} sensitivity is higher than 5 in reactor R5).

The slowly biodegradable substrate (X_S) is sensitive to the hydrolysis rate constant k_H and the hydrolysis saturation constant K_X in all the reactors because the ASM3 model, in contrast to ASM1, does not distinguish between hydrolysis under anoxic and aerobic conditions, i.e. ASM3 does not include the anoxic reduction factor η_h.

As expected, the storage rate constant (k_{STO}) has a strong influence on the S_S concentration. However, a comparatively much lower effect – or no effect at all – on the other component concentrations is observed, including the S_{O2} and the X_{STO} concentrations, which are consumed and produced, respectively, during the aerobic storage of S_S. The latter can be explained by the relatively low concentration of S_S available in the system compared to e.g. X_{STO}, as the corresponding Monod factors also reflect (see Table 3). A dosage of an external carbon source as control actuator would definitively improve the system performance. This fact will be considered further in the section on sensitivity analysis upon control handles. This case illustrates a way of using the Monod factors and the sensitivities for model/process analysis.

The kinetic rate expressions of seven of the 12 biological processes modeled in the ASM3 model involve the concentration of heterotrophs (X_H). Therefore, an appreciable effect of the maximum specific growth rate of heterotrophic biomass (μ_H) on several model component concentrations is expected. Nevertheless, the sensitivity analysis only shows a high value for X_{STO}, the storage component that is the substrate for biomass growth in ASM3.

In the above parameter sensitivity analysis the individual effect of each parameter has been analyzed. For model calibration, however, it is important to realize which parameter groups are most sensitive and how the parameter sensitivities interrelate. Such information can be obtained from analysis of the parameter covariance matrix, which is formed from the parameter sensitivity matrix as: $\mathbf{V}=\mathbf{S}^T\mathbf{S}$.

The parameter covariance matrix may be analyzed using principal component analysis (PCA) to determine which linear combination of parameters affects the variance most and then also which linear combination of parameters affects the variance second most, etc. This information is contained in the orthogonal principal components.

The sensitivity analysis is presented for the static case to illustrate differences between the two models. If a calibration is to be carried out, clearly it is also important to include dynamic information.

Model sensitivity to control handles. Relative sensitivity

The most interesting results are obtained from the sensitivity analysis carried out for a number of potential control handles that can theoretically be used to optimize the operation of a N removal plant. Here it is important to realize that the normalized static sensitivities are equal to the normalized static gains for each actuator. Five different control handles were evaluated: the internal (nitrate) recycle flow rate ratio, the external (sludge) recycle flow rate ratio, the oxygen transfer rate through adjustment of the K_La coefficient, the waste sludge flow rate and, finally, dosage of an external carbon source into the anoxic zone (R1). The value of each control handle (parameters in the model's equation system) assigned in the reference simulation was also perturbed in +0.01% to perform the study. The sensitivities of the model component concentrations to the control handles for both models are presented in Table 6. Table 7 includes the relative sensitivity, which, for a particular model component, is defined as the ratio between its sensitivity in the ASM3 model to that in the ASM1 model. (Only the model components present in both models are listed.) A negative relative sensitivity implies an opposite response of both models, which can be important for simulation-based control structure evaluation. Especially the slowly biodegradable substrate (X_S) shows negative relative sensitivities to four of the five control handles, indicating an opposite response of both models to those control handles.

Internal (nitrate) recycle flow rate ratio From Table 6 it seems that an increase of the internal (nitrate) recycle flow rate is not desirable, since it will considerably increase the S_{O2} and S_{NOX} concentrations in the anoxic zone. The former will cause a detrimental effect on the process efficiency, and the latter, which was already high for the reference simulation, is pointless from a treatment point of view since no readily biodegradable substrate (S_S) is available. The ASM1 model is more sensitive than the ASM3 model with respect to the S_{NOX} component, but both models show essentially the same S_{O2} sensitivity in the anoxic zone. In fact, under the given circumstances it can be concluded that a decrease of the nitrate recycle flow rate could save on pumping costs

Table 6. ASM1 and ASM3 model sensitivity analysis to control handles

Ranges: <0.1; 0.1-0.5; 0.5-1.5; 1.5-3.0; >3.0

		Control handles																								
		Internal recycle rate ratio					Aeration rate					External carbon dosage					Waste sludge flow rate					Sludge recycle flow rate				
		Reactor					Reactor					Reactor					Reactor					Reactor				
Comp	ASM	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
S_S	1	-	-	-	+	+	-	-	-	-	-	+	+	0	-	-	+	+	+	+	+	-	-	-	-	-
	3	-	-	+	0	0	-	-	-	-	-	+	+	-	-	-	+	+	+	+	+	-	-	-	-	-
X_I	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	-	-	-	-	+	+	+	+	+
	3	0	0	0	0	+	+	0	+	0	+	+	0	+	0	+	-	-	-	-	-	+	+	+	+	+
X_S	1	-	-	-	+	+	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+
	3	-	0	0	0	+	0	+	+	0	+	-	-	0	-	-	+	+	+	+	+	-	0	0	-	0
X_H	1	0	0	0	0	0	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+
	3	0	0	0	0	-	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+
X_A	1	0	0	0	0	0	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+
	3	0	0	0	0	0	+	+	+	+	+	0	0	0	0	0	-	-	-	-	-	+	+	+	+	+
S_{O2}	1	+	+	0	0	+	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+	+	+	-	-	-
	3	+	+	0	0	+	+	+	+	+	+	-	-	-	-	-	+	+	+	+	+	-	-	-	-	-
S_{NOx}	1	+	+	+	+	0	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+
	3	+	+	+	0	0	+	+	+	+	+	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+
S_{NH4}	1	-	-	-	-	+	-	-	-	-	-	-	-	+	+	+	+	+	+	+	+	-	-	-	-	-
	3	-	-	-	-	+	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	-	-	-	-
S_{ALK}	1	-	-	-	-	0	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	-	-	-	-
	3	-	-	-	0	0	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	-	-	-	-

Table 7. Relative sensitivities (ASM3 to ASM1 sensitivity ratio)

Ranges
<0.6
0.6-0.95
0.95-1.05
1.05-1.4
1.4-2.0
>2.0

Control handles	Internal recycle rate ratio					Aeration rate					External carbon dosage					Waste sludge flow rate					Sludge recycle flow rate				
	Reactor					Reactor					Reactor					Reactor					Reactor				
Comp.	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
S_S	+	+	-	0	0	-	+	+	+	-	+	+	D	+	+	+	+	+	+	+	+	+	+	+	+
X_I	D	D	D	D	D	D	D	D	D	D	D	D	D	D	D	+	+	-	-	+	+	+	-	-	+
X_S	+	0	0	0	+	0	-	-	0	-	-	-	0	-	-	-	-	-	-	-	-	0	0	-	0
X_H	D	D	D	0	D	D	D	D	D	D	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
X_A	D	D	D	D	D	+	+	+	+	+	0	0	0	0	0	+	+	+	+	+	+	+	+	+	+
S_{O2}	+	+	D	D	+	+	+	+	+	+	-	-	+	+	+	+	+	+	+	+	-	-	+	+	+
S_{NOx}	+	+	+	0	D	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
S_{NH4}	+	+	+	+	+	+	+	+	-	+	-	-	+	+	+	+	+	-	+	+	+	+	-	+	+
S_{ALK}	+	+	+	0	D	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

while not resulting in a significant decrease of the effluent quality.

Dosage of an external carbon source into the anoxic zone The dosage of an external carbon source into the anoxic zone is another factor that influences the denitrification process. It has a significant effect on the S_{NOX} concentration in all five reactors of the simulated treatment plant. In the second anoxic reactor, the S_{NOX} sensitivity reaches values up to 2.7 and 2.3 for the ASM1 and ASM3 models, respectively. This means that the denitrification process efficiency is substantially improved by the carbon source addition. The sensitivity values decrease and become comparable towards the end of the treatment ($\approx$1 for both models). Since an external readily biodegradable substrate is fed to the system, an increased consumption of S_{O2} associated with biomass growth takes places. Clearly, S_S is lacking in the influent wastewater, and external carbon source dosage could result in an important improvement of the effluent quality.

Sludge recycle flow rate ratio An increase of the sludge recycle flow rate results in increased biomass concentration in the treatment plant. The ASM3 model exhibits higher sensitivity values for both groups of organisms than the ASM1 model. However, this increased biomass concentration in the activated sludge tanks is not desirable since it will result in higher oxygen consumption (with a notably stronger effect on the ASM3 model predictions), and closely related to that, higher aeration costs. Moreover, the load on the sedimentation tank will increase, and the pumping cost will increase too. However, the analysis results of both models also indicate that the increased sludge concentrations are especially beneficial for the nitrification process, since X_A increases more (relatively) compared to X_H for an increase of the sludge recycle ratio. This tendency is observed in both models but the ratio between the sensitivity of X_A and X_H is about 2 for all the reactors using the ASM1 model and varies from 1.6 to 2 for the ASM3 model, depending on each reactor. The relative sensitivity values (Table 7) indicate that the ASM3 model is more sensitive to this control handle on the autotrophic (X_A) and heterotrophic (X_H) biomass than the ASM1 model. The S_{NH4} relative sensitivity value is higher than 1 for the anoxic zone and the first aerobic reactor, essentially 1 for the second aerated reactor and less than 1 at the end of the treatment. According to the model, as the individual S_{NH4} sensitivities are negative, the effluent S_{NH4} concentrations benefit from the increased sludge recycle ratio.

Waste sludge flow rate Increasing the waste sludge flow rate, an important effect can be observed on the S_{NH4} sensitivity in both models, mainly in the aerobic zone (values >1). This large value is because a lower concentration of nitrifying organisms is present in the system when the waste sludge flow rate is increased. Accordingly, an important influence on the S_{O2} sensitivities is observed. Besides the reduced amount of X_A, the decreased amount of X_H will also affect the S_{O2} concentration. A decrease of the waste sludge flow rate will be beneficial for the nitrification process. In fact, with respect to X_A and S_{NH4}, a reduction of the waste sludge flow rate seems more effective than the sludge recycle rate ratio as a control action to improve nitrification in the treatment plant under study.

Oxygen transfer rate (K_La **coefficient**) Regarding the oxygen transfer rate, Table 7 shows that for the same change on the oxygen transfer coefficient (K_La), the ASM3 model predicts a higher improvement of the nitrification performance compared to the ASM1 model. The S_{NOX} relative sensitivity is around 1.5 for R1, R2 and R3, and even higher for R4 and R5. Relative sensitivities lower than 1 for S_{O2} and from almost 1 to above 1.7 for S_{NH4} also reflect this fact. It should be noted that S_{NOX} and S_{NH4} have positive and negative sensitivities, respectively, since S_{NOX} is produced during nitrification whereas S_{NH4} is consumed. The analysis of the Monod factor values (Table 3) also indicated that ASM3 predicted a higher limitation of the nitrification process by S_{O2} compared to ASM1. Thus, for the nitrification process, the plant is under-designed regarding the oxygen transfer rate. Both models show high (individual) sensitivities for all the model components involved in the nitrification process over the whole reaction zone.

The relative importance of the possible control handles can be evaluated through a PCA analysis of the actuator covariance matrix. Here, this is carried out for the static actuator covariance analysis.

Dynamic behavior towards disturbances of the biological N removal treatment plant using ASM1 and ASM3 models

In order to investigate some aspects of the biological N removal dynamics, the responses of the ASM1 and ASM3 models to pulse- and step-type disturbances on the model input component specifications and potential actuators for control are analyzed. The analysis is carried out using reference parameters for both models, and starting from the steady state conditions listed in Table 2.

Pulse-type disturbance

Usage of a pulse disturbance means that the static process gain from the influent disturbance to the effluent concentration is equal to the area under the response curve divided by the input pulse area, if a single disturbance is used. Hence, this ratio equals the static gain, which is equal to the static sensitivity.

Disturbance on the wastewater input specifications

Figure 3 shows the responses predicted by the ASM1 and ASM3 models when the influent slowly biodegradable substrate concentration (X_S) is doubled for 1 h at the beginning of day 2 of the simulation run. The magnitude of this disturbance is comparable to the peak X_S concentration reached during the storm weather scenario of the COST benchmark (Copp 2002).

The simulated X_S and S_S effluent concentration patterns are qualitatively similar for both models (Fig. 3a and b), albeit that the influence of the disturbance lasts much longer for the ASM3 model. The latter is probably related to the lower hydrolysis rate in the ASM3 model, as mentioned before. Quantitatively, however, the responses are very different when the different scales are taken into account. There is also a significant qualitative difference on the effluent S_{NH4} predictions between the two models for this case study (see Fig. 3c and d). The ASM1 and ASM3 models show an opposite response on the predicted S_{NH4} concentrations. Like disturbing X_S, a pulse disturbance on the influent S_S concentration shows the same dynamic behavior (results not shown).

The explanation for the differences between the ASM1 and ASM3 model predictions relies on the different structure of both models. In the ASM1 model, increasing the influent slowly or readily biodegradable substrate concentrations (X_S and S_S, respectively) only leads to an increase of the total influent COD concentration. In the ASM3 model, a similar increase on the X_S or S_S load renders an increase of both the total influent COD and N concentrations, since the ASM3 model links a fraction of N to each influent COD fraction (in this case to X_S). Thus, the observed increase in effluent S_{NH4} concentrations for the ASM3 model is the result of an increase of the influent total N concentrations, whereas for the ASM1 model the decrease in effluent S_{NH4} concentrations is the result of the increased incorporation of S_{NH4} into biomass, growing on the extra S_S or X_S supplied. This observation also explains the significantly different relative sensitivity for S_{NH4} (see Table 7).

The disturbance on the readily biodegradable substrate S_S can, in fact, also be considered as a dosage of an external carbon source into the anoxic zone, where the

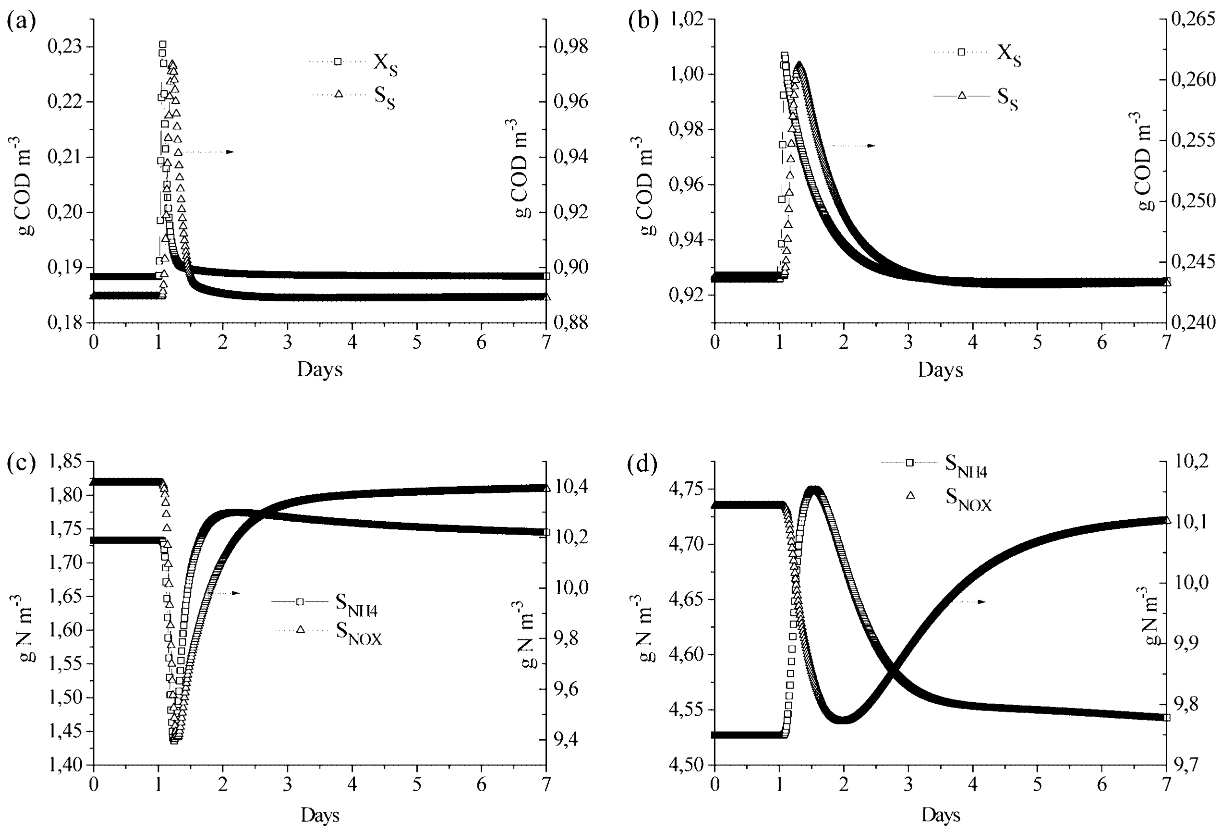

Fig. 3a–d. Pulse disturbance on influent X_S. Effluent slowly biodegradable substrate X_S (**a**, **b**: left axis), readily biodegradable substrate S_S (**a**, **b**: right axis), ammonium S_{NH4} (**c**, **d**: left axis) and nitrate S_{NOX} (**c**, **d**: right axis) for the ASM1 model (**a**, **c**) and the ASM3 model (**b**, **d**)

denitrification process takes place. Denitrification requires carbonaceous matter as electron donor to proceed at reasonable rates. Since the hydrolysis of X_S releases S_S, Fig. 3c and d shows the beneficial effect of the X_S disturbance on the denitrification process predicted by both models while the perturbing effects are still acting on the system.

Finally, Fig. 4 shows the response for the ASM1 and ASM3 models, respectively, when a pulse disturbance of 30% increase on the influent S_{NH4} concentration is applied for 1 h at the beginning of day 2 of the simulation run.

Both models show qualitatively similar patterns for both effluent S_{NOX} and S_{NH4} components. In this case, only the influent total N concentration was increased during the pulse disturbance, contrary to the disturbance on X_S previously described, where both influent total COD and total N were increased simultaneously. Thus, similar trends are observed for both models as response to the S_{NH4} influent pulse disturbance. Again, the effect of the disturbance is much longer for the ASM3 model.

Disturbances on the control handles

In this subsection, the dynamic response of the model effluent N components to pulse disturbances on the $K_L a$ coefficient (oxygen transfer rate), the sludge and nitrate recycle flow rate ratios are analyzed. In the previous section a disturbance on the influent S_S concentration was already evaluated, and can be considered also as a pulse disturbance on an external carbon source supply (as a control handle).

Oxygen transfer rate ($K_L a$ coefficient). The COST $K_L a$ coefficient values for all aerated reactors were increased by 50% for 1 h. Figure 5a and b shows the S_{NH4} and S_{NOX} responses predicted by the ASM1 and ASM3 models, respectively. The patterns observed for both models are rather similar, i.e. the S_{NH4} concentration decreases whereas the S_{NOX} concentration increases due to the disturbance. Clearly, an improvement of the nitrification process is observed while the disturbing effect of extra S_{O2} is still acting on the system.

Nitrate recycle flow rate ratio. A nitrate recycle flow rate ratio change from 3.0 to 4.0 (1.33 times the COST default value) was applied for 1 h. Figure 6a and b shows the responses of the S_{NH4} and S_{NOX} concentrations predicted by the ASM1 and ASM3 models, respectively. The response of the model output (S_{NH4} and S_{NOX} concentrations) is completely different compared to the response to the $K_L a$ modification: for both models the effluent S_{NH4} concentration quickly increases during the disturbance. As soon as the nitrate recycle flow rate ratio returns to its original value, the effluent S_{NH4} concentrations quickly decrease, and even reach values below the steady state

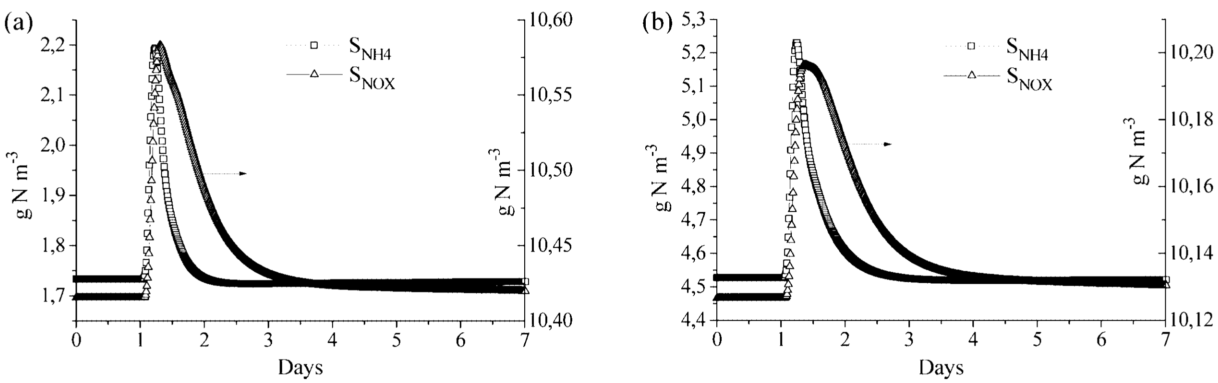

Fig. 4a, b. Pulse disturbance on the influent S_{NH4} concentration. Effluent ammonium S_{NH4} (**a**, **b**: left axis) and nitrate S_{NOX} (**a**, **b**: right axis) for the ASM1 model (**a**) and ASM3 model (**b**)

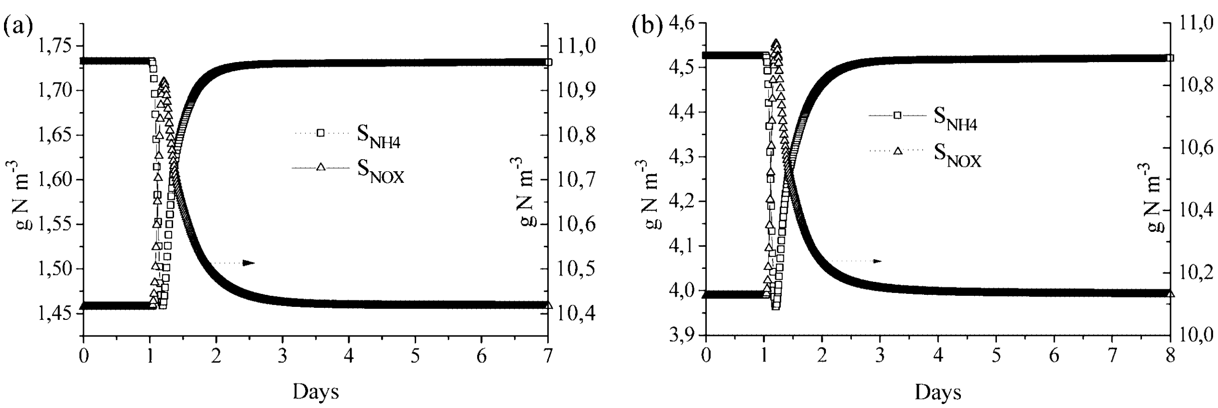

Fig. 5a, b. Response of effluent ammonium S_{NH4} (**a**, **b**: left axis) and nitrate S_{NOX} (**a**, **b**: right axis) for the ASM1 model (**a**) and the ASM3 model (**b**) to a pulse disturbance on the oxygen transfer rate ($K_L a$ value)

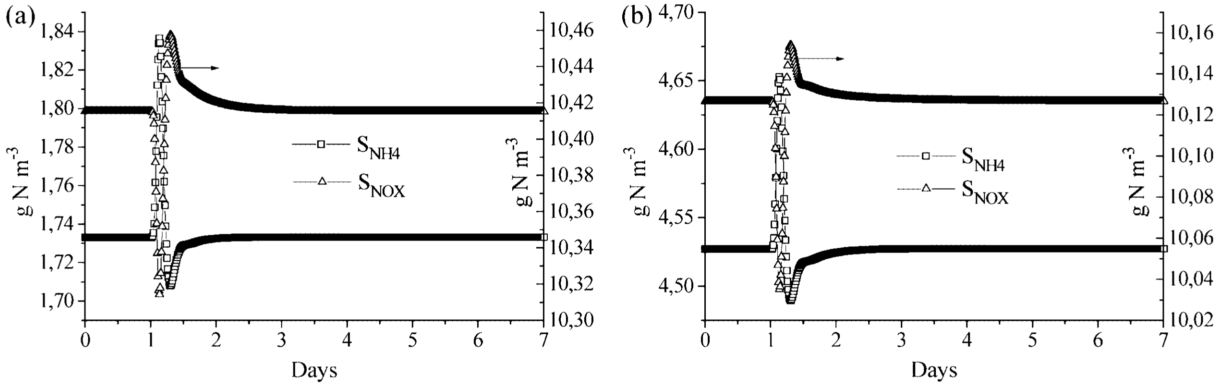

Fig. 6a, b. Response of effluent ammonium S_{NH4} (**a, b**: left axis) and nitrate S_{NOX} (**a, b**: right axis) for the ASM1 model (**a**) and ASM3 model (**b**) to a pulse disturbance on the nitrate recycle flow rate ratio

effluent S_{NH4} concentration. Finally, the effluent S_{NH4} values slowly return to their steady state values. Similar patterns are observed for S_{NOX}. Again, the ASM3 model requires more time than the ASM1 model to reach steady state after the pulse disturbance.

Sludge recycle flow rate ratio. In this case, 1.5 times the COST default value for the sludge recycle flow rate ratio (from 1.0 to 1.5) was imposed for 1 h as pulse disturbance. Figure 7a and b shows the predicted S_{NH4} and S_{NOX} responses of the ASM1 and ASM3 models respectively. The ASM3 model requires more time than ASM1 to recover the steady state condition. The response of the ASM1 model to this disturbance is similar to that for the nitrate recycle ratio pulse disturbance (see Fig. 6a).

Step-type disturbance

Disturbances on the control handles

Sludge recycle flow rate ratio. A 50% increase of the sludge recycle flow rate ratio was applied. The predicted responses for the ASM1 and ASM3 model are shown in Fig. 8.

A significant difference between the step responses obtained with both models can be observed. The ASM1 model has a very fast initial transient in the opposite direction to the final static change. Thereafter there follows a slower transient also in the wrong direction compared to the final static change. The ASM3 model has initially a very strong and slow transient in the wrong direction, which after about 2 weeks moves in the direction of the final static value. Note that the final, i.e. the static, gain is much smaller for the latter model than for the ASM1 model. The dynamic response for both models can be explained as follows.

The step increase of the sludge recycle flow rate ratio will decrease the average liquid residence time of the mixed liquor present in the activated sludge tanks. It means that there is less time for nitrification, and accordingly, the S_{NH4} concentrations increase almost instantaneously following the step disturbance, resulting in the very fast initial transient in Fig. 8. Similarly, the S_{NOX} concentrations decrease instantaneously, because nitrate is the end product of the nitrification process. Both models show an inverse response for ammonium as well as nitrate. It takes a long time, i.e. around four liquid mean residence times, to reach the new steady state. The behavior predicted by both models is rather different, especially for nitrate. Both models predict that the effluent S_{NH4} concentration evolves slowly to a new steady state. The step disturbance will in the long term modify the sludge distribution between the secondary settler and the activated sludge tanks. As a consequence, the concentration of autotrophic bacteria (X_A) in the activated sludge

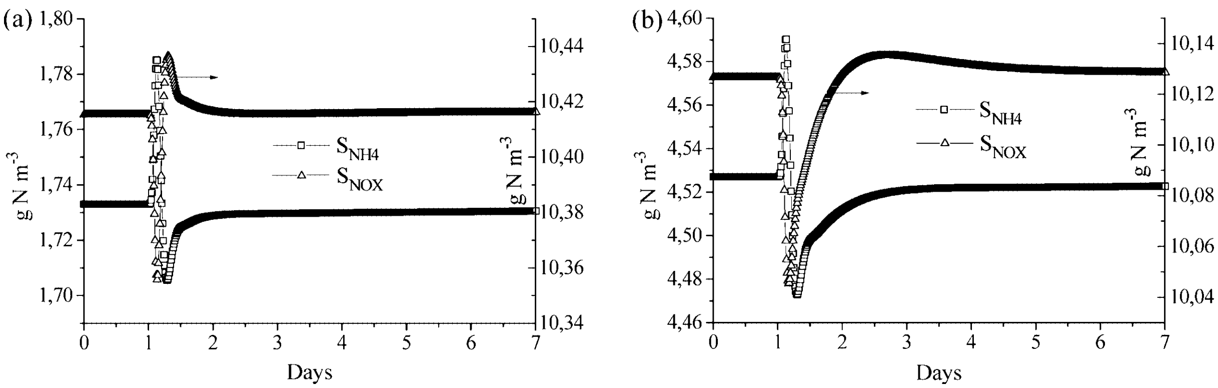

Fig. 7a, b. Response of effluent ammonium S_{NH4} (**a, b**: left axis) and nitrate S_{NOX} (**a, b**: right axis) for the ASM1 model (**a**) and ASM3 model (**b**) to a pulse disturbance on the sludge recycle flow rate ratio

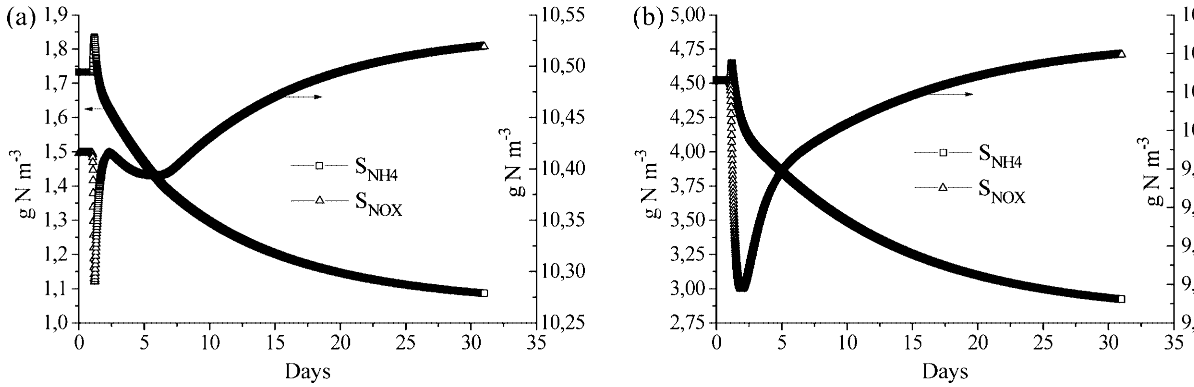

Fig. 8a, b. Response of effluent ammonium S_{NH4} (**a**, **b**: left axis) and nitrate S_{NOX} (**a**, **b**: right axis) for the ASM1 model (**a**) and ASM3 model (**b**) to a 50% step increase of the sludge recycle flow rate ratio

system will change. The latter is a very slow process, mainly due to the low specific growth rate of the autotrophic bacteria (μ_A), which explains why it takes such a long time to reach the new steady state for both effluent S_{NH4} and S_{NOX} concentrations. For nitrate, the slower transient in the opposite direction compared to the final static direction predicted by the ASM1 model is probably due to an increase of the denitrification efficiency. The latter is due to more hydrolysis taking place at the increased sludge concentrations in the activated sludge tanks.

This wrong way or inverse response behavior of the sludge recycle flow rate ratio implies that efficient usage of this control handle requires a multivariable control design.

Nitrate recycle flow rate ratio. As step disturbance, 1.33 times the COST default value for the nitrate recycle flow rate ratio (from 3.0 to 4.0) was imposed.

The nitrate recycle flow rate ratio exhibits a distinct wrong way or inverse response for both models. The static gain is clearly lower for the ASM3 model, whereas the inverse response is stronger. The dynamic response for both models can be explained as follows.

The increase of the nitrate recycle flow ratio will also decrease the average liquid residence time of the mixed liquor in the activated sludge tanks. The very fast transient in the effluent ammonium profile is more pronounced than in Fig. 8, since the decrease of the average liquid residence time is more drastic for the disturbance depicted in Fig. 9. Both models predict an increase of the effluent ammonium concentrations for the new steady state. For nitrate, both models show an inverse response. The nitrate concentration at the new steady state is higher than the nitrate concentration obtained for the original steady state. The increase of the nitrate concentration in the final steady state is probably the effect of the introduction of more oxygen in the anoxic zone via the nitrate recycle flow, resulting in a reduced overall denitrification efficiency of the activated sludge system.

As in the previous case, this wrong way behavior of the nitrate recycle flow rate ratio implies that efficient usage of this control handle requires a multivariable control design.

Summarizing, both ASM1 and ASM3 are rather complex models. The ASM3 model structure is more transparent and, as a consequence, ASM3 simulation results are easier to interpret, mainly due to the simpler cell decay model principle in ASM3 (endogenous respiration).

It is clear from the simulation of the disturbance scenarios that the dynamics in both models are quite different. For both models an inverse response for nitrate was obtained for the sludge and nitrate recycle flow rate ratios when step-type disturbances were introduced. The ASM3 model usually requires a longer time than the ASM1 model to reach steady state when a disturbance is imposed on the steady state conditions. In this respect, Koch et al.

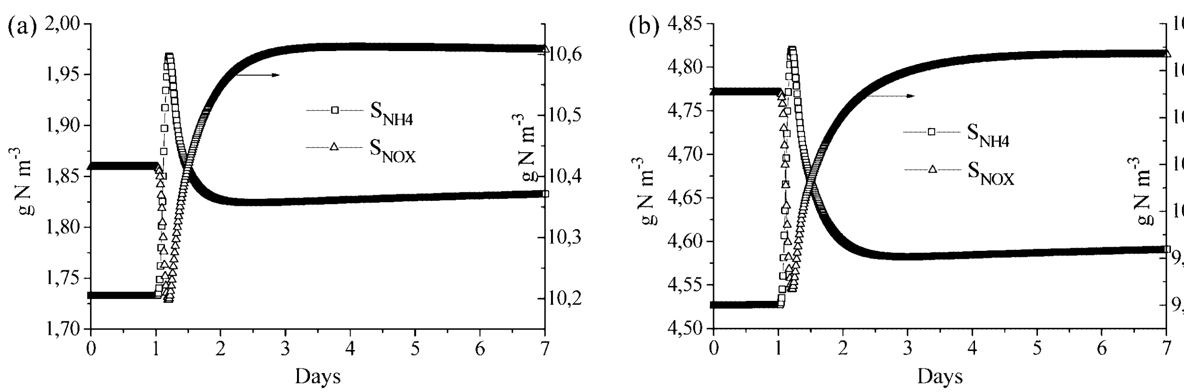

Fig. 9a, b. Response of effluent ammonium S_{NH4} (**a**, **b**: left axis) and nitrate S_{NOX} (**a**, **b**: right axis) for the ASM1 model (**a**) and ASM3 model (**b**) to a 33% step increase of the nitrate recycle flow rate ratio

(2000) concluded that the ASM3 model provides a closer agreement with experimental results than ASM1 in situations where the storage of readily biodegradable substrate is dominating, e.g. in batch tests, or during periods of high COD loads in full-scale wastewater treatment plants caused by significant diurnal influent flow rate and COD concentration variations, or for plants with substantial non-aerated zones.

The modeling purpose of control strategy implementation on an N removal plant is reflected in the dynamic response to actuator moves and in the static sensitivities. This combined information may be used for designing experiments, which focus on comparing the model behaviors thus facilitating model falsification and model parameter estimation.

Conclusions

A predenitrification benchmark plant was analyzed using the ASM1 and ASM3 models. For a similar N and COD load, the steady state effluent concentrations predicted by both models showed some distinctive differences that could to a large extent be explained by differences in the model concepts.

The steady state system performance was analyzed by evaluating the Monod factor values and by performing a static sensitivity analysis to the model kinetic parameters. Both methods complement each other. This analysis provides insights into the influence of specific model parameters on the system performance. In this way, a reduction of the number of parameters subject to determination from experimental data can be achieved.

The steady state system response to manipulation of the potential control handles was evaluated via a sensitivity analysis. The concept of relative sensitivity was introduced to quantify the relative effect of each actuator on the model predictions for the two models. The negative relative sensitivities of the slowly biodegradable substrate (X_S) to four of the five control handles analyzed imply an opposite response of the two models, which can be rather important for control structure design.

The analysis of the process behavior to pulse and step disturbances showed that the dynamics in both models are different. The ASM3 model usually requires a longer time than the ASM1 model to reach steady state. ASM3 simulation results are easier to interpret because the model structure is more transparent, mainly due to the simpler cell decay in ASM3. An inverse response was obtained for the sludge and nitrate recycle flow rate ratios, indicating that multivariable control design is required.

Clearly, it is of utmost interest to evaluate the performance of the ASM3 model on a realistic wastewater treatment plant. This paper pinpoints specific differences between the two models. In an experimental investigation these differences should be focused upon in order to facilitate model falsification.

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