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An extended Benchmark Simulation Model n°2 with processes for nitrous oxide emission and side-stream pH-dependent partial nitritation/Anammox treatment

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Summary of key findings

Benchmark Simulation Models n°1 and n°2 are tools enabling the development and the unbiased comparison of control strategies applied for wastewater treatment systems. According to new emerging control objectives, such as nitrous oxide (N_2O) emission mitigation and high side-stream nitrogen removal, the Benchmark Simulation Model n°2 is extended during the present work. In particular, the Activated Sludge Model for Greenhouse gases n°1 is used to include the N_2O production in the mainstream while the Complete Autotrophic Nitrogen Model to describe the processes for a side-stream partial nitritation/Anammox reactor. In this last model a pH calculation is included. A benchmark simulation model, the Benchmark Simulation Model n°2 for Nitrous oxide and pH-dependent Complete Autotrophic Nitrogen Removal, enabling the development and test of control strategies not only ensuring good effluent quality but also low nitrous oxide emissions and high nitrogen removal efficiency is obtained.

Background and relevance

Benchmark simulation models, such as the Benchmark Simulation Models n°1 and n°2 (BSM1 and BSM2), are tools developed with the aim of providing a reference simulation platform where control strategies aiming at high wastewater treatment (WWT) performance can be designed and tested in an unbiased and realistic way. In particular, the BSM1 uses a plant layout of predenitrification and a secondary settler whereas the BSM2 adds the wastage sludge treatment to this configuration (Gernaey, Jeppsson, Vanrolleghem, & Copp, 2014). Although the BSM2 enables the development and testing of a large number of control strategies, there are features which need to be further updated in response to new emerging WWT control objectives (Jeppsson et al., 2013). Among these, the mitigation of nitrous oxide emissions and the enhancement of cost-efficient side-stream nitrogen removal are particularly required. According to these exigencies, two extensions of the BSM2 are performed in this work. For the first extension, the Activated Sludge Model for Greenhouse gases n°1 (ASMG1) by Guo and Vanrolleghem (Guo & Vanrolleghem, 2014) is used in the mainstream activated sludge (AS) unit replacing thereby the Activated Sludge Model n°1 (ASM1). As an outcome, the Benchmark Simulation Model n°2 for Nitrous oxide (BSM2N) is obtained. Secondly, the plant layout is extended with a PN/A treatment unit as a side-stream treatment of the ammonium-rich effluent from the anaerobic digester. To this end, the Complete Autotrophic Nitrogen Removal (CANR) model by Vangsgaard *et al.* (Vangsgaard, Mauricio-Iglesias, Gernaey, Smets, & Sin, 2012) is employed to describe the processes occurring in a single-stage granular reactor. As process performance fluctuates in response to varying pH, a pH calculation routine is included for the CANR model. As a result, this study provides an extension of the Benchmark Simulation Model n°2 for Nitrous oxide and pH-dependent Complete Autotrophic Nitrogen Removal (BSM2NpluspH-CANR).

Materials and methods

Extension of the BSM2 with processes for nitrous oxide production in the mainstream

The model used to include the N_2O production and emission from the mainstream is the ASMG1 by Guo & Vanrolleghem (2014). The model was calibrated and validated across the ASM1 in order to fit the liquid concentrations. However there is no validation of the dynamics of N_2O predicted by the model. The ASMG1 splits out the ASM1 nitrification into the two following steps: the aerobic ammonium oxidation by ammonia-oxidising bacteria (AOB) and the aerobic nitrite oxidation by nitrite-oxidising bacteria (NOB). On the other hand, the one-step heterotrophic denitrification is split out into four sequential steps by taking into account the production and the subsequent consumption of nitrite, nitric oxide and nitrous oxide, namely the nitrate-to-dinitrogen reduction intermediates. Furthermore, two-step nitrifier denitrification is used to describe the production of N_2O by AOB. Extensions of the pre-existing interfaces, which are tools mapping a set of state variables of a model into the ones of another model, had to be carried out in order to map the ASMG1 state variables into the ones of the Anaerobic Digester Model n°1 and vice versa.

Extension of the BSM2 with side-stream partial nitritation/Anammox treatment units

As mentioned in the introduction, a reactor for one-stage continuous granular-based PN/A treatment is added in the side-stream line following the dewatering unit of the anaerobically-digested wastage sludge. A first tentative volume of this reactor was determined on the basis of an influent nitrogen volumetric ratio of 750 mg $N.L^{-1}.d^{-1}$. As the nitrogen content in the water rejected from the dewatering unit changes when the CANR reactor is introduced, a sequence of iterations was performed before determining the right volume. Afterwards a safety factor was introduced to allow good performance efficiencies when using dynamic influent. A value of 400 cubic meters for the volume resulted.

The model used for the process description is illustrated in detail in Vangsgaard et al. (2012). A pH calculation is implemented into the model in order to take into account the important interdependence between CANR processes and pH. The pH is calculated by solving the following electronic charge balance equation:

$$-2 \cdot HCO_3^- \cdot \frac{KeHCO3}{H^+} - HCO_3^- - \frac{K_w}{H^+} + H^+ - NO_3^- - TNN \cdot \frac{KeHNO2}{KeHNO2 + H^+} + TAN \cdot \frac{H^+}{H^+ + KeNH4} + Z^+ = 0 \qquad (1)$$

In Eq. (1) KeHCO3, KeHNO2, K_w and KeNH4 are equilibrium constants for bicarbonate, nitrous acid, water and ammonium. HCO_3^-, NO_3^-, TNN (total nitrite nitrogen), TAN (total ammonia nitrogen), Z^+ (i.e. background charge) and H^+ are used as molar concentrations ($mol.L^{-1}$). Since the CANR model splits the granule biofilm from the centre to the extreme into 99 layers and then considers the bulk separately, a value of H^+ is found for each of the layers and the bulk by solving Eq. (1) by means of the bisector method. To speed up the calculations performed in MATLAB/Simulink, the pH was calculated iteratively: at the first step the model calculates all the state variables in the granule layers and in the bulk using an initial guess of the pH. The solutions are then used in Eq. (1) to find a value of pH which is used as guess for the next step. The time interval between two consecutive steps is chosen as a result of a trade-off between the need for high calculation accuracy, given by very short intervals, and computation speed, given by larger intervals. A value of 10^{-6} days was selected as a good compromise.

When implementing the new reactor into the plant-wide configuration, new interfaces mapping the ASMG1 state variables into the ones of the CANR model and vice versa needed to be modelled. Moreover, AnAOB were included as new state variables in the mainstream line.

Results and discussion

The BSM2NpluspH-CANR (Figure 1) was simulated by controlling the oxygen concentration in the last three AS reactors of the mainstream at 0.5 - 1 - 2 mg (- COD).L^{-1}. Steady-state simulations were performed and the results were analysed in order to study the impact of the inclusion of the new nitrogen removal reactor on the N_2O emissions from the mainstream unit and the reliability of the novel pH calculation implemented for the CANR reactor.

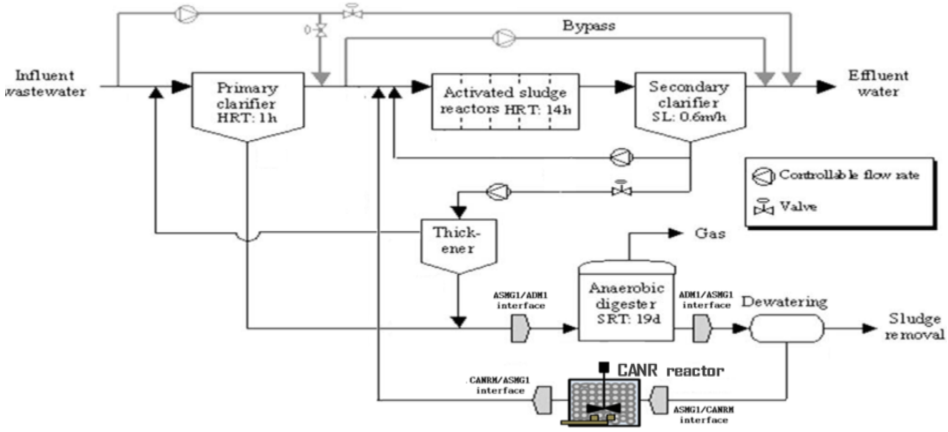

Figure 1.1: Layout of the Benchmark Simulation Model n^{o}2 for Nitrous oxide and pH-interdependent Complete Autotrophic Nitrogen Removal.

Impact of the inclusion of the CANR reactor on the mainstream N_2O emissions

In order to study the effect on the emissions of N_2O from the mainstream when the CANR reactor is included, emission factors of N_2O from the five mainstream biological tanks are calculated with respect to the TN load in the inlet to the activated sludge (AS) unit. To explain the differences in the emissions predicted by BSM2N and BSM2NpluspH-CANR, the N_2O production and consumption rates by HB and AOB specific to the TN in the AS unit inlet are calculated and evaluated as well. From Table 1 it can be noted that there is a significant reduction in the N_2O emission factors (around 40%) from the mainstream when the new CANR reactor is included. This reduction is expected and the underlying reasons can be explained as a function of the three main mechanisms contributing to the N_2O emission: stripping, heterotrophic anoxic activity and AOB activity. With regard to the stripping, it is a remarkable fact that, when the new reactor is included, the oxygen mass transfer rate, manipulated by the oxygen controller, is lower. The reason for this is that in order to maintain the same oxygen concentration, less oxygen has to be supplied when the AS reactors receive a reduced nitrogen load. Consequently, the stripping of the N_2O produced by the different microorganisms is reduced. Reducing the stripping, in turn, means that there is more liquid N_2O available to be reduced by denitrifying activity of HB to N_2. With regard to the contributions by HB and AOB, the values of their specific rates are found to be lower when the side-stream treatment reactor is added. The reason for having lower AOB-mediated N_2O production is the fact that a lower concentration of AOB occurs as the fed nitrogen is reduced. In turn, a lower amount of nitrite and nitrate are produced for heterotrophic denitrification, which explains the lower production and consumption rates by HB. From these considerations it can be concluded that a lower specific amount of N_2O emitted from the mainstream can be achieved by including the side-stream treatment for CANR removal. This is because the side-stream reactor reduces the reactive TN influent load to the mainstream AS unit by 25%, which implicates less air supply demand and thus less mass transfer of liquid N_2O to the atmosphere.

Table 1.1: Emission factors and specific N_2O production and consumption rates by HB and AOB with regard to the TN load in the AS unit influent.

DO concentration	Specific N_2O production rate by HB		Specific N_2O consumption rate by HB		Specific N_2O production rate by AOB		Emission factors	
	BSM2N	BSM2NpluspH-CANR	BSM2N	BSM2NpluspH-CANR	BSM2N	BSM2NpluspH-CANR	BSM2N	BSM2NpluspH-CANR
g (-COD).m^{-3}	g N.m^{-3}.d^{-1}.g^{-1} $N_{IN,AS}$		g N.m^{-3}.d^{-1}.g^{-1} $N_{IN,AS}$		g N.m^{-3}.d^{-1}.g^{-1} $N_{IN,AS}$		[g N_2O-N_{emit}.g^{-1} $N_{IN,AS}$]	
0.5	2,56E-05	2,13E-05	-2,56E-05	-2,13E-05	1,59E-11	8,51E-12	3,75E-05	2,02E-05
1	2,48E-05	2,13E-05	-2,48E-05	-2,13E-05	1,25E-11	2,73E-12	1,79E-05	1,06E-05
2	2,40E-05	2,04E-05	-2,40E-05	-2,10E-05	1,98E-11	1,20E-11	1,91E-05	1,11E-05

The pH-dependent CANR reactor

In this section, the pH-dependent CANR reactor simulation results for oxygen concentration in the mainstream at 1 mg (-COD).L^{-1} are illustrated. In particular, steady-state simulation results have shown that the reactor operates with a TN removal efficiency of 88.5 % and a pH slightly less than 7. These results can be considered realistic when compared to the data collected by Lackner *et al.* (Lackner et al., 2014).

Figure 1.2 shows the profiles of the model state variables used to solve the charge balance and of the resulting pH profile within the granule. As can be noted from the molar concentration values of the different species, TAN is the predominant component in the charge balance calculation. As a result, the pH profile follows the same trend of TAN.

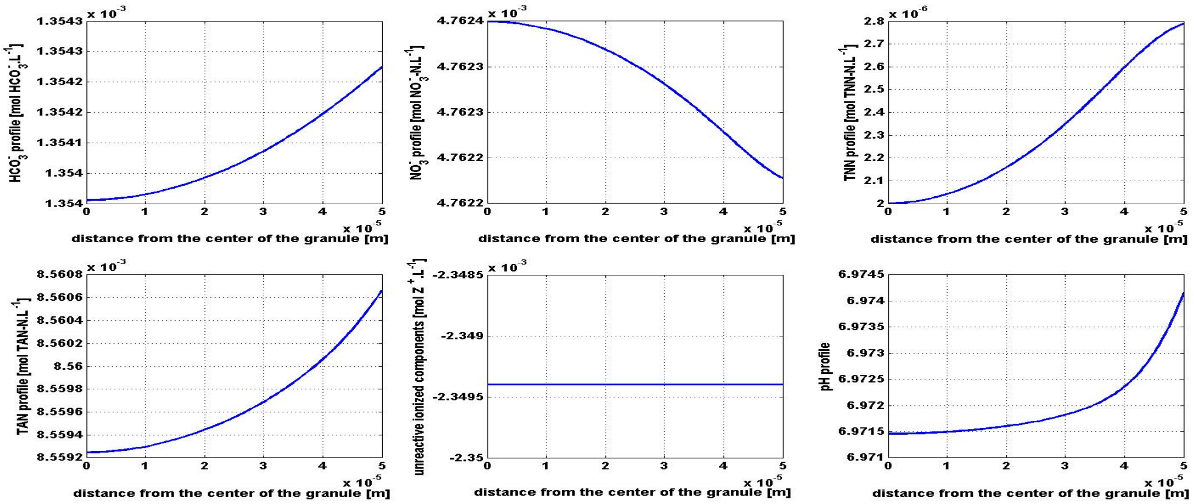

Figure 1.2: Steady-state granule profiles of the state variables involved in the charge balance and of the pH.

Conclusions

In this study two new benchmark simulation models have been built up: the BSM2N and the BSM2NpluspH-CANR. Simulation results have addressed how the inclusion of the new CANR treatment reduces the potential of the plant to emit N_2O from the mainstream for the same TN load treated. Furthermore the model has shown its capability to predict realistically the interdependence between pH and CANR processes. These benchmark models can therefore be used for future development and objective comparison of a wide number of novel control strategies aiming at both enhancing the biological treatment in the mainstream line and at reducing the N_2O emissions from the mainstream, and ensuring high process performance of the PN/A reactor.

References

Gernaey, K. V., Jeppsson, U., Vanrolleghem, P. A., & Copp, J. B. (2014). *Benchmarking of Control Strategies for Wastewater Treatment Plants*.

Guo, L., & Vanrolleghem, P. A. (2014). Calibration and validation of an activated sludge model for greenhouse gases no. 1 (ASMG1): prediction of temperature-dependent N2O emission dynamics. *Bioprocess and Biosystems Engineering*, *37*(2), 151–163. doi:10.1007/s00449-013-0978-3

Jeppsson, U., Alex, J., Batstone, D. J., Benedetti, L., Comas, J., Copp, J. B., … Vrecko, D. (2013). Benchmark simulation models, quo vadis? *Water Science and Technology : A Journal of the International Association on Water Pollution Research*, *68*(1), 1–15. doi:10.2166/wst.2013.246

Lackner, S., Gilbert, E. M., Vlaeminck, S. E., Joss, A., Horn, H., & van Loosdrecht, M. C. M. (2014). Full-scale partial nitritation/anammox experiences - An application survey. *Water Research*, *55*, 292–303. doi:10.1016/j.watres.2014.02.032

Vangsgaard, A. K., Mauricio-Iglesias, M., Gernaey, K. V, Smets, B. F., & Sin, G. (2012). Sensitivity analysis of autotrophic N removal by a granule based bioreactor: Influence of mass transfer versus microbial kinetics. *Bioresource Technology*, *123*, 230–241. doi:10.1016/j.biortech.2012.07.087