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Control of wastewater N_2O emissions by balancing the microbial communities using a fuzzy-logic approach

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Abstract: In this work, a fuzzy-logic controller for minimization of the nitrous oxide emission from wastewater treatment plants is developed and tested in a simulation environment. The controller is designed in order to maintain a balance between production and consumption of nitrite by AOB and NOB microorganisms respectively. Thus, accumulation of nitrite is prevented and AOB denitrification, the main N_2O producer, is drastically slowed down. The controller is designed to adjust the oxygen supply according to a measured parameter which typically indicates the ratio of the activity of NOB over AOB. The controller is tested on a benchmark simulation model describing the production of N_2O during both AOB denitrification and HB denitrification. Comparisons between simulation results of open-loop and closed-loop have revealed the potential of the controller to significantly reduce the amount of N_2O emitted (approximately 35%). On the other side, this reduction of N_2O was accompanied by an increase in the aeration costs. Moreover, a plant performance evaluation under dynamic disturbances shows that the effluent quality is compromised due to higher requirements of organic carbon by denitrifying heterotrophs. The controller can therefore be considered effective for the reduction of N_2O production by AOB but would need to be coupled with a secondary control strategy ensuring a complete oxidation of the nitrogen oxides by heterotrophs to have a good effluent quality.

Keywords: fuzzy-logic, benchmark, nitrous oxide emission, autotrophic denitrification, nitrogen, wastewater treatment plants (WWTPs).

1. INTRODUCTION

Nitrous oxide (N_2O) is well-known as an ozone-depleting substance and a harmful greenhouse gas with a global warming potential 300 times higher than carbon dioxide. Measurement campaigns at wastewater treatment plants (WWTPs) have revealed that a considerable amount of N_2O can be emitted [1,2]. Developing control strategies aiming at reducing its emissions becomes therefore of interest. During the biological WWT processes, N_2O is found to be produced by two different microbial groups: ammonia-oxidizing bacteria (AOB) and heterotrophic bacteria (HB) [3]. In particular, AOB have shown their capability in using the produced NO_2^- instead of O_2 as electron acceptor for the oxidation of NH_4^+. The reduction of NO_2^- carries N_2O as end product. Another possible pathway is the incomplete hydroxylamine oxidation by AOB. Intermediate compounds accumulated during this process can lead to N_2O. With regard to the role of HB, N_2O is produced as intermediate compound during the reduction of nitrogen oxides like NO_3^- and/or NO_2^- into N_2. If the reduction of N_2O into N_2 is slower than the reduction of those N oxides into N_2O, an accumulation of N_2O can occur. The minimization of N_2O emissions can therefore be achieved by slowing down both the AOB-mediated N_2O-production processes and the net HB-mediated N_2O production. Furthermore, operational costs have to be taken into account in order to evaluate the economic feasibility of the control implementation.

For the development of a control strategy applied to biological wastewater processes, a fuzzy-logic approach can be the most suitable to be adopted. As a matter of fact, given their interactive nature and their high non-linearity, biological wastewater treatments can be more suitably controlled by fuzzy-logic controllers than by linear controllers like the Proportional Integrative Derivative (PID) ones [4]. Furthermore, fuzzy-logic controllers (FLCs) present the additional possibility of incorporating expert knowledge about the processes to be controlled [5]. FLCs are also not affected by the capability of a mathematical model in describing realistically the processes to be controlled, since their design is independent from the model used. Furthermore, adopting a fuzzy-logic approach easily allows including the fuzziness associated with the control objectives, typically related to the WWT processes [6]. For these reasons, a FLC aiming at minimizing the N_2O emissions by balancing the activity of the different microbial groups is developed in the present work. In particular, MATLAB/Simulink is used as computer environment for the development of the fuzzy-logic control strategy. The model employed for testing its performance is the Benchmark Simulation Model N°2 for Nitrous oxide (BSM2N), developed by Boiocchi *et al.* [7]. On this platform, dynamic simulations will be performed in order to evaluate the

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capability of the controller in reducing the N_2O emissions and its contextual effect on effluent quality and operational costs.

2. MATERIALS AND METHODS

2.1 The Benchmark Simulation Model n°2 for Nitrous oxide

As mentioned in the introduction, the model on which the performance of the controller is tested is the Benchmark Simulation Model N°2 for Nitrous oxide (BSM2N), developed by Boiocchi *et al.* [7]. The model is an extension of the Benchmark Simulation Model N°2 (BSM2) by Jeppsson *et al.* [8]. It describes the physical and biochemical mainstream and side-stream processes occurring in a typical pre-denitrification WWTP. The virtual configuration of the BSM2N is presented in Figure 1. As can be seen, the biological mainstream unit consists of two well-mixed anoxic tanks (ANOX1 and ANOX2) followed by three aerated tanks (AER1, AER2 and AER3). The biological processes occurring in these reactors are described by an upgraded version of the Activated Sludge Model N°1 (ASM1) by Henze *et al.* [9], namely the Activated Sludge Model for Greenhouse gases N°1 (ASMG1) by Guo and Vanrolleghem [10]. The state variables of the ASMG1 are: oxygen (S_{O2}); readily-biodegradable and slowly-biodegradable carbon (S_S and X_S); ammonium, nitrite, nitrate, dinitrogen, nitric and nitrous oxide nitrogen (S_{NHx}, S_{NO2}, S_{NO3}, S_{N2}, S_{NO} and S_{N2O}); soluble and particulate inerts (S_I and X_I); soluble and particulate organic nitrogen (S_{ND} and X_{ND}); alkalinity (S_{ALK}); heterotrophic, ammonia-oxidizing and nitrite-oxidizing bacteria (X_{HB}, X_{AOB} and X_{NOB}). The processes included in the ASMG1 are: aerobic growth of X_{HB}; hydrolysis of X_S, hydrolysis of X_{ND}; ammonification of S_{ND}; aerobic growth of X_{AOB}; aerobic growth of X_{NOB}; anoxic growth of X_{HB} on S_{NO3}, on S_{NO2}, on S_{NO} and on S_{N2O}; anoxic growth of X_{AOB} on S_{NO2} and on S_{NO}; decay of X_{HB}, X_{AOB} and X_{NOB}. As can be noted, N_2O is modelled to be produced according to two pathways: during HB denitrification and during nitrite reduction (via nitric oxide) by AOB. On the other hand, the production of N_2O as a consequence of incomplete hydroxylamine (NH_2OH) oxidation by AOB is not included in the model. There is however a significant amount of full-scale experiences suggesting AOB denitrification instead of the incomplete NH_2OH oxidation as the main contributor of N_2O [1,11–15]. Furthermore, a recently-developed model including the incomplete NH_2OH reveals that the amount of N_2O possibly produced during this process would be rather low compared to the amount of N_2O produced during AOB and HB denitrification [16].

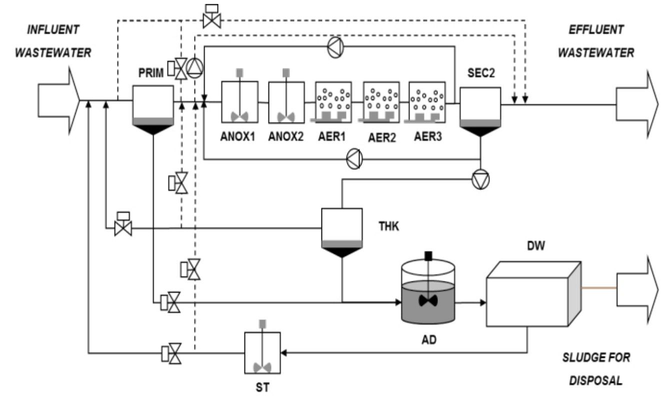


Figure 1: BSM2N layout [8].

2.2 Fuzzy-logic inference system

In this section, a brief overview of the work of a fuzzy-logic inference system is presented in order to allow a better understanding of the typical features needed to be decided when designing a fuzzy-logic controller. A fuzzy-logic inference system consists of the following three main sequential operations:

1) Fuzzification, where numerical (crisp) inputs are converted into linguistic (fuzzy) inputs, according to predefined membership functions (MFs),
2) Fuzzy inference, where fuzzy outputs are deduced on the basis of the fuzzy inputs deduced in point 1), according to specified linguistic rules,
3) Defuzzification, where fuzzy outputs are converted into numerical (crisp) outputs according to predefined MFs and a chosen defuzzification method.

As can be deduced, the main parameters to be decided during the design of a fuzzy-logic controller are the MFs of input and output variables and the linguistic rules linking input to output variables. Further details about the generic work of a fuzzy-logic inference system are given in Lababidi and Baker [17].

2.3 Definition of control structure

As mentioned in the introduction, the controller has to be designed in such a way that it minimizes the production of N_2O by both AOB and HB. Heterotrophic denitrification can only occur under low oxygen conditions. The process can therefore occur in the anoxic zone (ANOX1 and ANOX2) and at very poor oxygenation regimes in the aerobic zone (AER1, AER2 and AER3). The contribution on N_2O by HB however would be stronger in the aerobic zone due to the higher mass transfer capability. In the anoxic zone, the HB-produced N_2O stays in the liquid phase and thus is more likely to be reduced into N_2 rather than to strip.

With regard to the production of N_2O during AOB denitrification, it is well-established that low oxygen concentrations and/or high nitrite (NO_2^-) availability promote the use of NO_2^- itself by AOB as electron acceptor for the oxidation of ammonium (NH_4^+). Hence, for its minimization, in the aerobic zone the oxygen has to be in a sufficiently high concentration to enhance the consumption of the AOB-produced NO_2^- by the coexisting microbial group, namely NOB. Enhancing the NOB activity by means of oxygen supply increase would contextually minimize the amount of N_2O produced by HB [18]. Thus the control of R_{NatAmm} can result beneficial for the reduction of the N_2O produced by both AOB and by HB.

For these reasons, monitoring the NOB activity over the one of AOB has been identified as a potential strategy for the minimization of the production of N_2O. The variable identified to be controlled at this purpose is the ratio between the nitrate produced by NOB and the ammonium consumed by AOB (R_{NatAmm}) in the aerobic zone, expressed in Eqn. (1).

$$R_{NatAmm} = \frac{|(NO_3^-)_{IN} - (NO_3^-)_{OUT}|}{|(NH_4^+)_{IN} - (NH_4^+)_{OUT}|} \quad (1)$$

A value of R_{NatAmm} around 1 theoretically indicates that all the nitrite produced by AOB is subsequently consumed by NOB. If R_{NatAmm} is lower than 1, not all the AOB-produced NO_2^- is consumed by NOB. Thus NO_2^- starts accumulating in the system, which would in turn enhance AOB denitrification. This is a typical situation resulting from low oxygen availability. On the other side, values of the parameter significantly higher than 1 represent oxygen inhibition of heterotrophic denitrification, where an accumulation of HB-produced NO_2^- occurs. A too high oxygen supply would in part directly inhibit the HB-produced NO_2^- reduction and consume a larger amount of organic carbon needed by HB. In this scenario, the oxygen supply needs to be turned down to avoid that the accumulated NO_2^- to be reduced into N_2O.

In virtue of these considerations, the control strategy use measurements from the influent and effluent of the aerobic zone of NH_4^+ and NO_3^- for the calculation of R_{NatAmm}, namely the controlled variable. The oxygen mass transfer coefficient (k_La) is used as a manipulated variable since changes in the oxygen availability forms the only available actuator that is able to induce the due shift on NOB activity. The fuzzy-logic controller is implemented in the mainstream aerobic zone as depicted in Figure 2. As can be seen, the controller will use R_{NatAmm} as direct input variable and will deduce a scaled deviation of the oxygen mass transfer coefficient ($\Delta_S k_La$) as output variable. The latter will have a value between -1 and +1. $\Delta_S k_La$ is then multiplied by a scaling factor (SF_{kLa}) in order to obtain its physical dimension. The deviations of k_La are integrated in time and then added up to their respective nominal values.

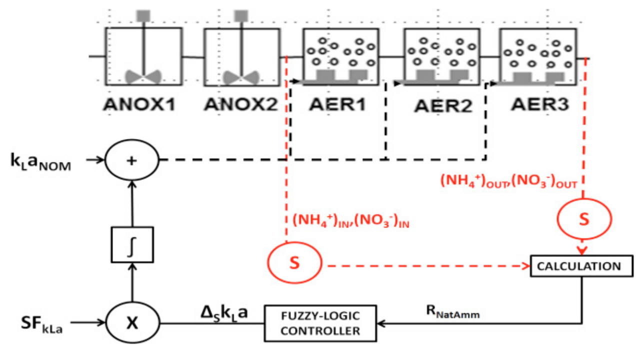
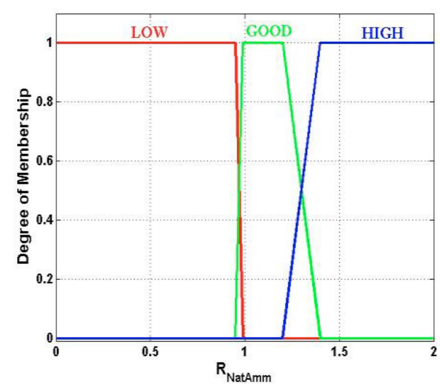


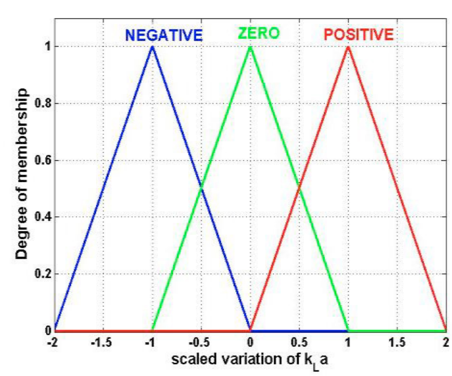
Figure 2: Block diagram for the implementation of the controller in the mainstream activated sludge unit.

2.4 Control tuning

The membership functions for the input and output variables are defined as represented in Figure 3 while Table 1 shows the linguistic rules to enable deducing, on the basis of the values of R_{NatAmm}, the variation of the k_La to be actuated on the three aerobic tanks. R_{NatAmm} is considered to be "GOOD" when it is comprised within 0.99 and 1.2. The reason for allowing a value of R_{NatAmm} slightly higher than 1 is due to the fact that a fraction of the incoming organic nitrogen, after being hydrolysed and ammonified, is usually oxidized into NO_2^- and then NO_3^-. An amount of NO_3^- higher than the NH_4^+ (i.e. R_{NatAmm}>1) consumed would therefore result. When R_{NatAmm} is in this range, no changes of k_La are designed to be actuated. On the contrary, the maximal positive change of k_La (i.e. $\Delta_S k_La$=+1) is decided to occur when R_{NatAmm} is equal or below 0.95, a scenario which would indicate that NOB need more oxygen for the conversion of NO_2^- into NO_3^- .When R_{NatAmm} is equal or higher than 1.4, inhibition of heterotrophic denitrification is considered to occur. In this case, the maximal negative change of k_La (i.e. $\Delta_S k_La$=-1) is defined to be inferred by the control system.



(a)



(b)

Figure 3: Membership functions for: (a) R_{NatAmm}, and (b) $\Delta_S k_La$.

Table 1: linguistic rules.

	IF	THEN
	R_{NatAmm}	$\Delta_S k_L a$
1	LOW	POSITIVE
2	GOOD	ZERO
3	HIGH	NEGATIVE

A value for the k_La_{NOM} equal to 120 d^{-1} is assigned for the first two aerobic reactors (AER1 and AER2) and a value of 60 d^{-1} was used for last tank (AER3), as prescribed by Jeppsson *et al.* [8]. 240 d^{-1}, namely the difference between the saturation limit of k_La (i.e. 360 d^{-1}) and the nominal value in the first two tanks (120 d^{-1}) is used as value for the scaling factor.

3. RESULTS

Simulations of the BSM2N open-loop and closed-loop are performed with the aim of addressing the changes due to the implementation of the novel control strategy. In particular, the BSM2N was simulated with a 609-day long dynamic influent by Jeppsson *et al.* [8], whose design details can be found in Gernaey *et al.* [19]. The dynamics and the steady-state of the influent Total Kjeldahl Nitrogen (TKN) load for the last month are depicted in Figure 4.

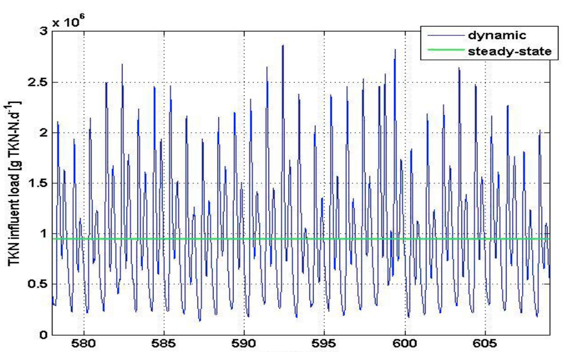


Figure 4: Dynamics and steady-state of influent TKN.

Corresponding to the same period of time, Figure 5 shows the dynamic results for both open-loop and closed-loop configurations of: (a) N_2O emission factor, calculated as percentage of N_2O emitted per unit of TKN in the influent, (b) R_{NatAmm}, (c) oxygen mass transfer coefficient of the first aerobic tank (AER1), and (d) the oxygen-to-nitrogen loading ratio (RO), calculated according to Eqn. (2) as the ratio between the oxygen supplied into the three aerobic tanks and the TKN in the influent of the first anoxic tank. The present quantity indicates the typical aeration regime of the plant.

$$RO = \frac{\sum_{i=1}^{3} V_i \cdot k_L a_i \cdot (S_{O,SAT} - S_{O,i})}{(S_{NH4,IN} + S_{ND,IN} + X_{ND,IN}) \cdot Q_{IN}} \tag{2}$$

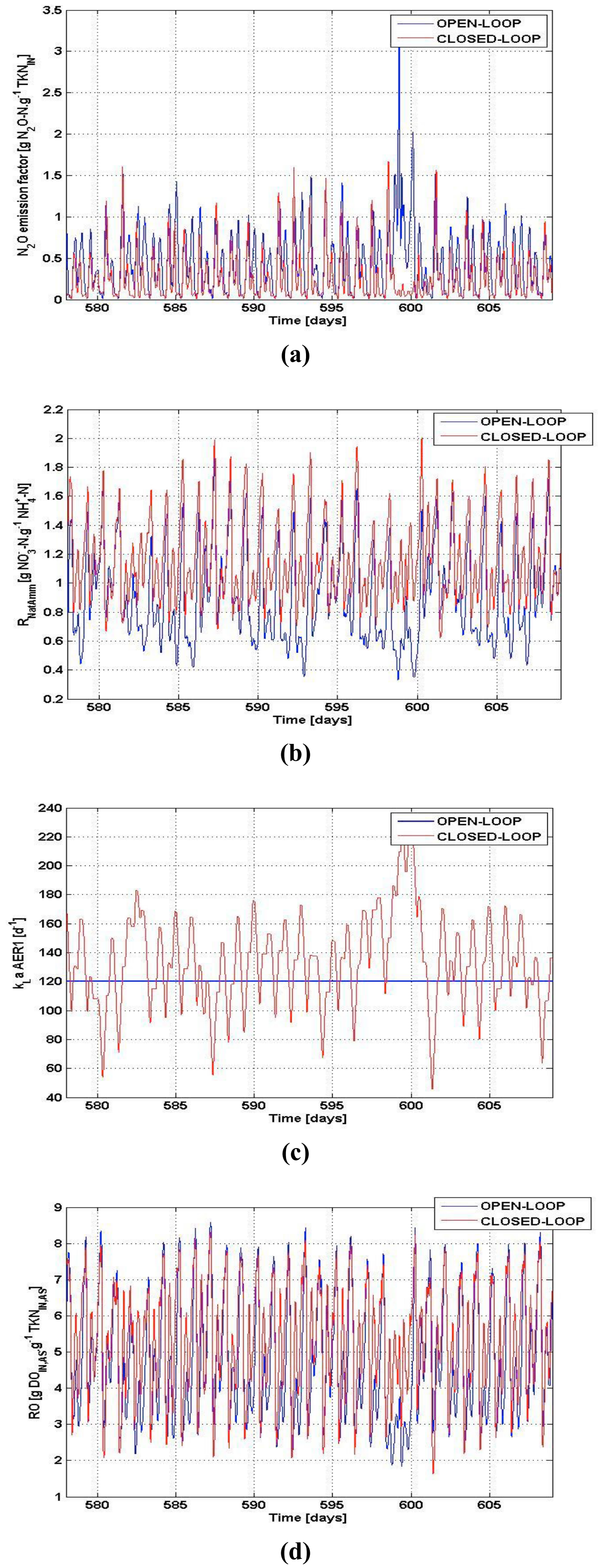


Figure 5: Last-month dynamics for: (a) N_2O emission factor, (b) R_{NatAmm}, (c) kLa of AER1, and (d) oxygen-to-nitrogen loading ratio.

Next, following the BSM2 protocol for the benchmarking of control strategies, from both the open-loop and closed-loop simulation results of the last 52 weeks, which allows a comparison more unbiased with regard to plant initial conditions and nominal value of k_La, the following average values are found:

- N_2O emission factors (N_2O_{ef}),
- total nitrogen removal efficiency (η_{TN}),
- R_{NatAmm},
- NO_2^- and NO_3^- effluent loads,
- Effluent limit violations in percentages of operating time for ammonium and total nitrogen (V_{NH4} and V_{TN}, respectively),
- Effluent Quality Index (EQI), calculated according to Jeppsson *et al.* [8] by taking into account the amount of the different pollutants in the effluent. The higher EQI is, the worst the effluent quality is,
- the average aeration energy (AAE), proportional to the oxygen mass transfer coefficients.

An overall evaluation of the impact of the controller implementation on the plant performance can thus be achieved. Table 2 summarizes the results.

Table 2: Open-loop and closed-loop plant performance evaluation.

	units	OPEN LOOP	CLOSED LOOP
N_2O_{ef}	[% g N_2O-N_{EM}.g^{-1} TKN-N_{IN}]	0.4	0.26
R_{NatAmm}	[g NO_3^--N.g^{-1} NH_4^+-N]	0.94	1.15
RO	[g $DO_{IN,AS}$.g^{-1} $TKN_{IN,AS}$]	4.7	5.3
$(NO_2^-)_{eff}$	[kg NO_2^--N.d^{-1}]	2.3	0.36
$(NO_3^-)_{eff}$	[kg NO_3^--N.d^{-1}]	167.6	269.1
η_{TN}	[% g TN_{REM}.g^{-1} TN_{IN}]	70.8	60.7
V_{NH4}	[% of operating time]	7.9	2.1
V_{TN}	[% of operating time]	2.2	12.8
EQI	[kg poll.units.d^{-1}]	5386.8	5650.3
AAE	[kWh.d^{-1}]	4026.7	5242

As can be noted, the controller is able to reduce the average N_2O emitted by 35% by keeping the controlled variable, namely R_{NatAmm}, at a higher value. Thus NOB activity is enhanced and, consequently, a higher consumption of NO_2^- results, leading to lower NO_2^- load in the effluent. However, due to the higher NOB activity, the load of NO_3^- in the effluent is drastically increased, which explains in turn the reduced TN removal efficiency (from 70.8% to 60.7%). The effluent quality index is therefore increased accordingly. Also the percentage of operating time in which TN violations (V_{TN}) are recorded is higher for the closed-loop configuration, although the percentage of operating time in which NH_4^+ violations (V_{NH}) occur is reduced due to the higher AOB resulting from the higher aeration. Since the controller has enhanced the NOB activity by increasing the amount of oxygen supplied, the average aeration costs have increased by approximately 30% compared to the open-loop case.

4. DISCUSSION

The results presented have shown the capability of the controller in reducing significantly the average amount of N_2O emitted by speeding up the NOB activity, which prevents the AOB-produced NO_2^- from being reduced to N_2O and . The results suggest that reduction in the total N_2O emitted, which can be considered satisfactory, can be improved by further enhancing NOB activity. On the other hand, enhancing the NOB activity meant also to decrease the effluent quality. As a matter of fact, when the AOB-produced NO_2^- was not subsequently oxidized into NO_3^-, heterotrophic denitrification worked more on NO_2^- and a lower amount of organic carbon was therefore needed compared to the case when the heterotrophic denitrification works on NO_3^-. Thus a more complete conversion of influent nitrogen in nitrogen gas and, consequently, a better effluent quality resulted in the open-loop.

It can therefore be concluded that the present fuzzy-logic controller, despite its effectiveness in minimizing N_2O emissions, is not sufficient alone in order to meet contextually the effluent nitrogen requirement. Hence, results suggest that a strategy controlling the TN removal efficiency is applied to the system as well in order to avoid compromising the effluent quality. With regard to this, one possible solution could be to add biodegradable organic carbon on top of the first anoxic tank (ANOX1) according to the amount of nitrogen oxides to be reduced. In alternative, the anoxic hydraulic retention time could be increased by manipulating the internal recycle flow rate.

5. CONCLUSIONS AND FUTURE PERSPECTIVES

A novel control strategy aiming at reducing the total amount of N_2O emitted from domestic wastewater treatment plants has been developed in this work. The control strategy is based on reducing nitrite accumulation, which would trigger the production of N_2O by both AOB and by HB. This is achieved by controlling in the aerobic zone the ratio between NOB-produced nitrate and AOB-consumed ammonium (R_{NatAmm}) at its optimal value, which was identified to be around 1. The oxygen mass transfer coefficient, directly proportional to the oxygen supply, was chosen as manipulated variable. The controller was built up in the simulation environment Simulink and then tested in the newly-developed Benchmark Simulation Model N^{o}2 for Nitrous oxide (BSM2N). The closed-loop simulation results were benchmarked against the open-loop results. The comparison revealed that the controller was able to effectively reduce the N_2O emissions by 35% by enhancing the NOB activity. At the same time effluent quality decreased drastically. It is therefore suggested that the present controller should be coupled with another controller for the achievement of a complete heterotrophic denitrification of nitrogen oxides either by regulating the amount of organic carbon externally added on top of the anoxic zone or by decreasing the internal recycle flow rate. Lastly, given the fact that the model does not include the N_2O-production pathway related to incomplete oxidation of hydroxylamine, the controller can be stated to be adequate only for the reduction of N_2O production during AOB and HB denitrification, which however can be considered the predominant N_2O contributors. Further evidences for the model description of the missing pathway need to be achieved.

Acknowledgements

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