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Modelling and control design for SHARON/Anammox reactor sequence

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Abstract: With the perspective of investigating a suitable control design for autotrophic nitrogen removal, this work presents a complete model of the SHARON/Anammox reactor sequence. The dynamics of the reactor were explored pointing out the different scales of the rates in the system: slow microbial metabolism against fast chemical reaction and mass transfer. Likewise, the analysis of the dynamics contributed to establish qualitatively the requirements for control of the reactors, both for regulation and for optimal operation. Work in progress on quantitatively analysing different control structure (pairing of controlled variables with manipulated variables) as well as exploring the feasibility of advanced process control including model predictive control.

Keywords: Autotrophic nitrogen removal, model predictive control, multivariable control, plantwide control, modelling

1. INTRODUCTION

Ammonium is one of the most abundant and important pollutants related with the waste water treatment, and should be removed before discharge, preventing problems for the biological media as eutrophication. As a consequence, ever more strict regulations set low nitrogen concentration thresholds for discharge. The first widely used process used for nitrogen removal consisted on nitrification and denitrification processes over nitrate. However, this process presents some disadvantage, namely high energetic consumption for oxygen supply, high tank volume and the need external carbon sources. A number of alternative operations for nitrogen removal have been developed in the last decades in order to reduce aeration costs, external carbon sources and sludge production the energy consumption, the footprint and the need of using carbon sources.

The SHARON process (Single reactor High activity Ammonia Removal Over Nitrite, Hellinga et al. 1998) was primarily based on the following sequences: i) the partial nitrification of the ammonium by aerobic oxidizing bacteria (AOB) and ii) the denitrification to nitrogen gas by heterotroph bacteria (HB).

Another option to this second step is the so-called anaerobic ammonium oxidation (Anammox, Murder et al.,1995). The process achieves a total ammonium conversion using equimolar amounts of ammonium and nitrite. This process presents some additional advantages, like the lowering of gases with greenhouse effect (CO_2 and NO_2) or the elimination of external carbon sources. Its main drawback is related to the low growth rate of Anammox bacteria, involving the use of sludge retention systems, e.g. membranes, granular systems. Besides, in order to achieve a high elimination of all the nitrogen sources, it must be

ensured that the ammonium and nitrite are fed in stable, close to equimolar proportions .

The partial nitrification can be achieved by a previous SHARON reactor coupled whit the Anammox process or both reactions can be implemented in a single reactor (CANON). In this case the SHARON-Anammox process is studied. The partial nitrification step:

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + H_2O + 2H^+$$
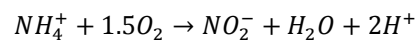
And the Anammox process follows the next equation:

$$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O$$
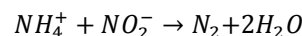
It has been reported that that with constant parameters, in the supposed corrects values, the ratio nitrite:ammonium might deviate from the ideal ratio and endanger the operation. Some strategies were applied in this field in order to optimize the nitrogen removal costs (Volcke et al. 2005). These strategies are based in different control loops, feedback and cascade, that fix set points for the key variables in the process, as pH or dissolved oxygen (DO), but always operating with them as independent loops. In order to get a better optimization of the global process and advanced control strategy is going to be applied. MPC (model predictive control) use the models of the process and predicts how is going to evolve it, and optimize at each time the set points of the individual control loops. Another objective is establish a procedure to configure and implement a MPC controller in different process, due nowadays there is no unification criteria to use them.

A scheme of the global waste water treatment plant is included in Appendix 2.

2. MODEL DEVELOPMENT

Both SHARON and Anammox reactor were modeled as continuous stirred tank reactors (CSTR). Assuming that the

reactor hold-up and all the inflows and outflows have the same constant density, the total mass and energy balances are:

$$\frac{dV}{dt} = F_{in} + F_{acid} + F_{base} + F_{CH_3OH} - F_{out} = F_{in,net} - F_{out} \tag{1}$$

$$\frac{d(V \cdot T)}{dt} = F_{in} \cdot T_{in} - F_{out} \cdot T_{out} - \frac{U_w \cdot \pi \cdot d_R \cdot H_R \cdot (T_{out} - T_{env})}{\rho \cdot C_P \cdot V} + \sum_j \frac{(-\Delta_R H)_j}{\rho \cdot C_P} \tag{2}$$

Additionally, it has been assumed that the Cp is equal and constant for every stream (2).

The individual mass balances developed are set up for the lumped compounds, because every change in a component involved in a chemical equilibrium causes changes in all the concentrations of all components that take part in the equilibrium. The individual mass balance for a component i is:

$$\frac{d(V \cdot C_i)}{dt} = F_{in,net} \cdot C_{i,in,net} - F_{out} \cdot C_i + k_L a_i \cdot (C_i^* - C_i) \cdot V + r_i \cdot V \tag{3}$$

The components considered are: H+, NH4+, NH3, HNO2, NO2-, CO2, HCO3-, CO32-, H2PO4-, HPO42-, NO3-, O2, N2, ammonia oxidizing bacteria (AOB), nitrite oxidizing bacteria (NOB), heterotrophic bacteria (HB), CH3OH and Z (charge not involved in biological reactions). Since some of the previous chemical species are in chemical equilibrium, the model works with lumped components, namely:

$$C_{TNH} = C_{NH_3} + C_{NH_4^+}$$

$$C_{TNO2} = C_{HNO_2} + C_{NO_2^{2-}}$$

$$C_{TIC} = C_{CO_2} + C_{HCO_3^-} + C_{CO_3^{2-}}$$

$$C_{TIP} = C_{HPO_4^{2-}} + C_{H_2PO_4^-}$$

2.1 Reaction modelling

Five different biological reactions are included in the SHARON model. The nitrification process is divided in two different steps: the oxidation of the ammonia to nitrite, carrying out by AOB, and the oxidation of the nitrite to nitrate, carrying out by NOB. The denitrification of both compounds is achieved by heterotrophic bacteria, as the oxidation of the methanol. The stoichiometric coefficients are showed in the Petersen matrix (tables 1 and 3). In order to take account of the microbial growth in the mass balances, the biomass composition is fixed as CH1.8O0.5N0.2.

The volumetric conversion rate for a component i is defined as:

$$r_i = \sum_{j=1}^{5} A_{ij} \cdot \rho_j \tag{4}$$

where Aij is the corresponding stoichiometric coefficient of the Pedersen matrix, and ρj is the process rate considered. The Pedersen matrix and the expressions of the process rates for the two reactors appear in the Appendix A.

2.2 pH calculation.

The microbial activity affects to the pH because exists a production and consumption of protons. These pH changes must be modeled in order to obtain the correct values during the reactor operation. In this case it is used a model based in a charge balance. The nonlinear system of equations is solved with a multidimensional Newton-Raphson method.

2.3 Gas-liquid transport

Gases are transported between both phases following the model showed below:

$$TR_i = k_L a_i \cdot (C_i^* - C_i) \tag{5}$$

The main gas in the process is the oxygen, and it'll be also a control variable of the process, so is the only modeled gas compound. With the Henry law the oxygen equilibrium concentration is obtained:

$$C_i^* = \frac{C_{G,i}^o}{m_i} \tag{6}$$

$$m_i = -403 + 2.52 \cdot T - 3.56 \cdot 10^{-3} \cdot T^2 \tag{7}$$

3. SIMULATION RESULTS

The models were tested using different cases study. For the SHARON reactor the conditions established in the simulations of A.Galí et al. in 2006 were used. This reactor is used to achieve a suitable influent for the Anammox reactor, with a ratio NO2-/NH4+ close to 1. With a hydraulic retention time of 1 day a removal efficiency of the 50% is achieved.
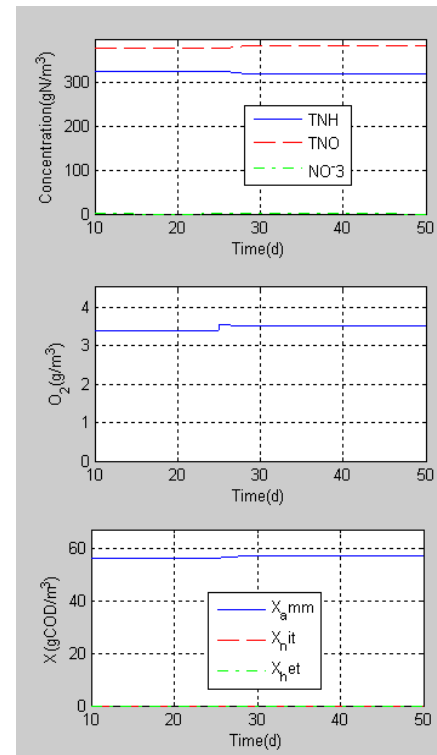

Figure 1: Simulation of $K_L a$ step of 5%

The response to-step inputs were also simulated to investigate the dynamics of the process. The first step consists in an increase of 5% in the $k_L a$ value. A higher growth rate is observed for AOB bacteria. In 5 days a new steady state is achieved. Two phenomena with different rates can be

observed. A peak is observed in the oxygen concentration because at the beginning of the step, corresponding to the higher oxygen mass transfer while the number of oxygen-consumming bacteria has not increased yet. As the bacteria concentration increases more ammonium is converted in nitrite and the concentration of oxygen decreases from the initial response.

With a decrease of 1% in pH the bacteria growth is lower, so they are in less concentration, while the oxygen level achieves higher values and the less ammonium is removed from the reject water. It is needed 11 days to achieve the new steady state.
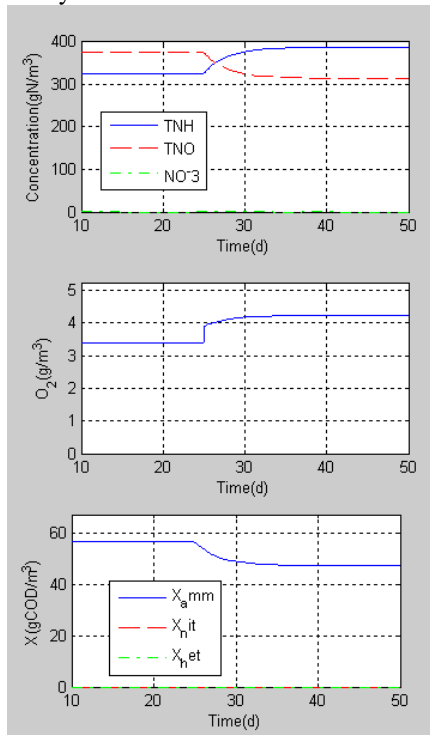

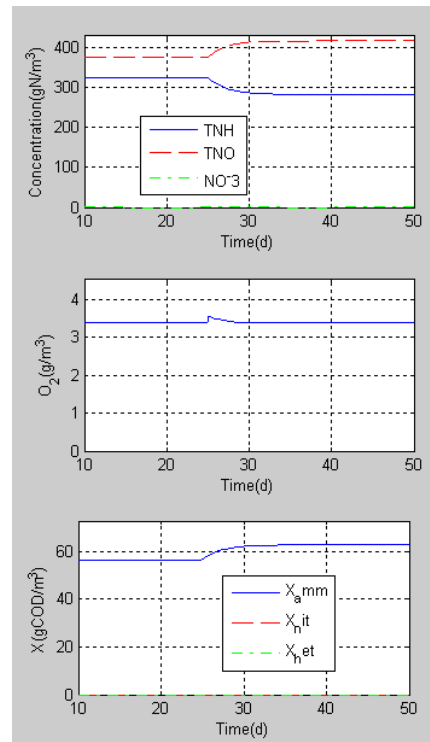**Figure 2: Simulation of pH step of -1%.**

Figure 3: Simulation of HRTstep of +5%.

Finally, the decrease of 5% of the output flow implies an increase of 5% of the hydraulic retention time, which allows a higher microbial growth of AOB. In 8 days the new steady state is achieved, with a decrease of the dissolved oxygen, because there are more bacteria consuming oxygen, but a peak is observed. This means that the DO has a faster response to flow changes than the bacteria concentration. Also a higher ammonium conversion is achieved.

The Anammox process was tested with the conditions used in the experiment of Güven et al. in 2004 in a lab-scale reactor. The ratio NO_2^-/NH_4^+ should be higher than 1 for stoichiometric reasons. Whit a hydraulic retention time of 5 days the ammonium removal efficiency is 94% and nitrite removal efficiency is higher than 99%. The overall nitrogen removal in the process is 90%.

6. CONCLUSIONS AND PERSPECTIVES

The main variable that links both reactors is the ratio NO2-/NH4+, which should be close to 1. The inspection of some step responses led to a qualitative screening of potential manipulated and controlled variables. For instance, pH should be controlled protons are produced because in the biological reaction driving the process to conditions out of the optimum range for the microbial growth. Another key parameter is the dissolved oxygen that has to be kept in a level that allows the growth of the AOB but prevents the growth of NOB or a too large conversion of ammonium. The hydraulic retention time play a similar role to oxygen as an intermediate value is needed to wash out the NOB but no the AOB. Temperature is also important because with low values, between 5-20 C, NOB growth faster than AOB. All this parameters can be controlled separately with different

feedback loops and fixed set points, but also cascaded structures can be used to actualize the set points when the ratio NO2-/NH4+ changes. Other possibilities are multivariable control strategies such as MPC. The implementation of an advanced control structure based on the modeling results will be investigated during future activities in this project.

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Appendix A. Reaction stoichiometry and expressions

Appendix B. Waste Water Treatment Plant with a SHARON-Anammox process.

Appendix A. Reaction stoichiometry

Table1. Gujer matrix of the SHARON process

j process	Aij												
	TNH	TNO2	CO2	TIP	NO3	O2	N2	AOB	NOB	Xhet	Methanol	H+	H2O
Ammonium oxidation	$-\dfrac{1}{Y_1}$	$\dfrac{1}{Y_1} - n$	-1			$-(-1 + \dfrac{1.5}{Y_1} - \dfrac{h}{4} + \dfrac{o}{2} - \dfrac{3}{4}\cdot n)$		1				$\dfrac{2}{Y_1} - n$	$\dfrac{1}{Y_1} - \dfrac{h}{2} + \dfrac{n}{2}$
Nitrite oxidation	-n	$-\dfrac{1}{Y_2}$	-1		$\dfrac{1}{Y_2}$	$-(-1 + \dfrac{0.5}{Y_1} - \dfrac{h}{4} + \dfrac{o}{2} + \dfrac{3}{4}\cdot n)$			1			n	$\dfrac{3}{2}\cdot n - \dfrac{h}{2}$
Denitrification nitrite	-n	$-\dfrac{1}{Y_3}$	$-\dfrac{1}{3} + \dfrac{0.5}{Y_3} - \dfrac{h}{6} - \dfrac{o}{3} - \dfrac{n}{2}$				$\dfrac{0.5}{Y_3}$			1	$-(\dfrac{2}{3} + \dfrac{0.5}{Y_3} + \dfrac{h}{6} - \dfrac{o}{3} - \dfrac{n}{2})$	$-\dfrac{1}{Y_3} + n$	$\dfrac{4}{3} + \dfrac{13}{6\cdot Y_3} - \dfrac{h}{6} - \dfrac{2\cdot o}{3} + \dfrac{n}{2}$
Denitrification nitrate	-n		$-\dfrac{1}{3} + \dfrac{5}{6\cdot Y_4} + \dfrac{h}{6} - \dfrac{o}{3} - \dfrac{n}{2}$		$-\dfrac{1}{Y_4}$		$\dfrac{0.5}{Y_4}$			1	$-(\dfrac{2}{3} + \dfrac{5}{6\cdot Y_4} + \dfrac{h}{6} - \dfrac{o}{3} - \dfrac{n}{2})$	$-\dfrac{1}{Y_4} + n$	$\dfrac{4}{3} + \dfrac{13}{6\cdot Y_4} - \dfrac{h}{6} - \dfrac{2\cdot o}{3} + \dfrac{n}{2}$
Methanol oxidation	-n		$-1 + \dfrac{1}{Y_5}$			$-(-1 + \dfrac{1.5}{Y_5} - \dfrac{h}{4} + \dfrac{o}{2} + \dfrac{3}{4}\cdot n)$				1	$-\dfrac{1}{Y_5}$	n	$\dfrac{2}{Y_5} - \dfrac{h}{2} + \dfrac{3}{2}\cdot n$

Table 2: Biological growth rate expressions of the SHARON process.

$$\rho_1 = \mu_{\max}^{AOB} \frac{C_{NH_3}}{K_{NH_3}^{AOB} + C_{NH_3}} \cdot \frac{C_{O_2}}{K_{O_2}^{AOB} + C_{O_2}} \cdot \frac{K_{I,HNO_2}^{AOB}}{K_{I,HNO_2}^{AOB} + C_{HNO_2}} \cdot X_{AOB}$$

$$\rho_2 = \mu_{\max}^{NOB} \frac{C_{HNO_2}}{K_{HNO_2}^{NOB} + C_{HNO_2}} \cdot \frac{C_{O_2}}{K_{O_2}^{NOB} + C_{O_2}} \cdot X_{NOB}$$

$$\rho_3 = \mu_{\max}^{dNO2} \frac{C_{TNO2}}{K_{NO_2}^{dNO2} + C_{TNO2}} \cdot \frac{K_{I,O_2}}{K_{I,O_2} + C_{O_2}} \cdot \frac{C_{TNO2}}{C_{TNO2} + C_{NO_3}} \cdot \frac{C_{CH_3OH}}{C_{CH_3OH} + K_{CH_3OH}^{het,an}} X_{het}$$

$$\rho_4 = \mu_{\max}^{dNO3} \frac{C_{NO_3}}{K_{NO_3}^{dNO3} + C_{NO_3}} \cdot \frac{K_{I,O_2}}{K_{I,O_2} + C_{O_2}} \cdot \frac{C_{NO_3}}{C_{TNO2} + C_{NO_3}} \cdot \frac{C_{CH_3OH}}{C_{CH_3OH} + K_{CH_3OH}^{het,an}} X_{het}$$

$$\rho_5 = \mu_{\max}^{met} \cdot \frac{C_{O_2}}{K_{O_2}^{het} + C_{O_2}} \cdot \frac{C_{CH_3OH}}{C_{CH_3OH} + K_{CH_3OH}^{het,ox}} X_{het}$$

Table 3: Gujer matrix of the Anammox process.

j process	Aij												
	TNH	O2	TNO2	NO3	N2	alk	S	XAOB	XNOB	XAnAOB	Xhet	Xs	Xi
AOB growth	$-\dfrac{1}{Y_{AOB}} - i_{NXB}$	$-\dfrac{3.43 - Y_{AOB}}{Y_{AOB}}$	$\dfrac{1}{Y_{AOB}}$			$-\dfrac{1}{14}\left(\dfrac{2}{Y_{AOB}} + i_{NXB}\right)$		1					
NOB growth		$-\dfrac{1.14 - Y_{NOB}}{Y_{NOB}}$	$-\dfrac{1}{Y_{NOB}}$	$\dfrac{1}{Y_{NOB}}$		$-\dfrac{i_{NXB}}{14}$			1				
AnAOB growth	$-\dfrac{1}{Y_{AnAOB}} - i_{NXB}$		$-\dfrac{1}{Y_{AnAOB}} - 1.52$	1.52	$\dfrac{2}{Y_{AnAOB}}$	$-\dfrac{i_{NXB}}{14}$				1			
AOB decay						$\dfrac{1}{14}(i_{NXB} - i_{NXI})$		-1				1-fi	fi
NOB decay						$\dfrac{1}{14}(i_{NXB} - i_{NXI})$			-1			1-fi	fi
AnAOB decay						$\dfrac{1}{14}(i_{NXB} - i_{NXI})$				-1		1-fi	fi
het1 growth	$-i_{NXB}$	$-\dfrac{1-Y_{het}}{Y_{het}}$					$-\dfrac{1}{Y_{het}}$				1		
het2 growth	$-i_{NXB}$		$-\dfrac{1-Y_{het}}{1.71Y_{het}}$		$\dfrac{1-Y_{het}}{1.71Y_{het}}$		$-\dfrac{1}{Y_{het}}$				1		
het3 growth	$-i_{NXB}$			$-\dfrac{1-Y_{het}}{2.86Y_{het}}$	$\dfrac{1-Y_{het}}{2.86Y_{het}}$		$-\dfrac{1}{Y_{het}}$				1		
het decay											-1	1-fi	fi
Hydrolysis	$-\dfrac{i_{NXB} - fi * i_{NXI}}{1 - fi}$						1					-1	

Table 4: Biological growth rate expressions of the Anammox process.

$$\rho_1 = \mu_{max}^{AOB} \frac{C_{NH_3}}{K_{NH_3}^{AOB} + C_{NH_3}} \cdot \frac{C_{O_2}}{K_{O_2}^{AOB} + C_{O_2}} \cdot \frac{K_{I,HNO_2}^{AOB}}{K_{I,HNO_2}^{AOB} + C_{HNO_2}} \cdot X_{AOB}$$

$$\rho_2 = \mu_{max}^{NOB} \frac{C_{HNO_2}}{K_{HNO_2}^{NOB} + C_{HNO_2}} \cdot \frac{C_{O_2}}{K_{O_2}^{NOB} + C_{O_2}} \cdot X_{NOB}$$

$$\rho_3 = \mu_{max}^{AnAOB} \cdot \frac{C_{HNO_2}}{K_{HNO_2}^{AnAOB} + C_{HNO_2}} \cdot \frac{K_{I,O_2}^{AnAOB}}{K_{I,O_2}^{AnAOB} + C_{O_2}} \cdot \frac{C_{NH_3}}{K_{NH_3}^{AnAOB} + C_{NH_3}} \cdot X_{NOB}$$

$$\rho_4 = b_{AOB} \cdot X_{AOB}$$

$$\rho_5 = b_{NOB} \cdot X_{NOB}$$

$$\rho_6 = b_{AnAOB} \cdot X_{AnAOB}$$

$$\rho_7 = \mu_{max}^{met} \cdot \frac{C_{O_2}}{K_{O_2}^{het} + C_{O_2}} \cdot \frac{C_S}{C_S + K_S^{het}} \cdot \frac{C_{TAN}}{C_{TAN} + K_{TAN}^{het}} \cdot X_{het}$$

$$\rho_8 = \mu_{max}^{het} \cdot \eta_H \cdot \frac{C_{TNH}}{K_{TNH}^{het} + C_{TNH}} \cdot \frac{K_{I,O_2}^{het}}{K_{I,O_2}^{het} + C_{O_2}} \cdot \frac{C_{TNO2}}{C_{TNO2} + C_{NO_3}} \cdot \frac{C_S}{C_S + K_S^{het}} X_{het}$$

$$\rho_9 = \mu_{max}^{dNO3} \cdot \eta_H \cdot \frac{C_{NO_3}}{K_{NO_3}^{het} + C_{NO_3}} \cdot \frac{K_{I,O_2}^{het}}{K_{I,O_2}^{het} + C_{O_2}} \cdot \frac{C_{TAN}}{K_{TAN}^{het} + C_{TAN}} \cdot \frac{C_S}{C_S + K_S^{het}} \cdot X_{het}$$

$$\rho_{10} = b_{AnAOB} \cdot X_{AnAOB}$$

$$\rho_{11} = k_H \cdot \frac{X_S}{K_X}$$

Appendix B. Waste Water Treatment Plant with a SHARON-Anammox process:

Influent

Activated sludge reactor

Secondar y settler

Effluent

Waste sludge

Return sludge

Treated reject water

Annamox

SHARON

$NO_2^-/NH_4^+=1$

Reject water

Sludge thickening, digestion, dewatering

Dewatered sludge

Possible external C-source