MODELLING THE SHARON PROCESS IN VIEW OF COUPLING WITH ANAMMOX

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Abstract: The combined SHARON-Anammox process for treating wastewater streams with high ammonia load, is discussed. Partial nitrification at high temperatures in a continuously aerated SHARON reactor, should yield an optimal ammonium/nitrite ratio, that is subsequently sent to the Anammox process to form nitrogen gas. A mathematical model of the SHARON process is presented. The stoichiometric matrix is formulated in terms of yield coefficients and biomass composition. Special attention is given to the calculation of pH. Preliminary simulations of the behaviour of the SHARON reactor are discussed. *Copyright © 2002 TiASWiK*

Keywords: Environmental engineering, Equilibrium, Mathematical models, Simulation, Steady State, Waste Treatment

1. INTRODUCTION

Partial nitrification techniques have been denoted for quite a while as very promising for improving sustainability of wastewater treatment (Abeling & Seyfried, 1992). The realization of nitrification/denitrification with nitrite as intermediate is beneficial both in terms of oxygen consumption, translated into reduced aeration energy costs, and COD-source addition costs, with savings of respectively 25% and 40% compared to traditional nitrification/denitrification via nitrate. Up till now, the SHARON (Single reactor High activity Ammonia removal Over Nitrite) process is the only reported process in which partial nitrification of ammonium to nitrite is successfully maintained in practice over a long time period (Mulder *et al.*, 2001). The SHARON process was developed more than five years ago at the Delft University of Technology. Microbial kinetic and stoichiometric parameters for ammonia oxidation were determined under the actual process conditions by lab-scale (1.5 l) tests (Hellinga

et al., 1999). Making use of both these experimental data and literature, the development of a dynamical process model in Matlab/Simulink for the classical SHARON reactor operated with heterotrophic denitrification, was started in view of further process design and scale-up (Hellinga *et al.*, 1999). The insights gained by simulations allowed the immediate design and construction of a full-scale process without the need for costly and time consuming intermediate pilot tests. The full-scale process is operational since January 1999 at the Rotterdam Sluisjesdijk sludge treatment plant. Full scale experience with the SHARON process has recently been described by Mulder *et al.* (2001) and van Kempen *et al.* (2001).

Recently, the coupling of the SHARON process with a so-called Anammox (anaerobic ammonia oxidation) process, in which ammonium and nitrite are converted to nitrogen gas under anaerobic conditions by autotrophic bacteria, finds more and more support in the search for sustainable wastewater treatment tech-

niques (van Dongen *et al.*, 2001a). Benefits of the combined SHARON-Anammox process compared to the SHARON process with denitrification are the reduction by 50% of the aeration costs, since only half of the ammonium is converted to nitrite, the omission of the need for additional COD source, the virtual absence of sludge production and the possibility to obtain low nitrogen effluent concentrations through the subsequent autotrophic Anammox reaction. The latter has been an inspiring starting point for the development of more sustainable municipal wastewater treatment systems (Jetten *et al.*, 1997). Processes like CANON (Hao, 2001; Hao *et al.*, 2001) and OLAND (Kuai and Verstraete, 1998), that combine partial nitrification and Anammox in one reactor, are currently also being studied.

An experimental study on the treatment of ammonium rich wastewater by the combined SHARON-Anammox process performed by van Dongen *et al.* (2001a), showed that the combined SHARON-Anammox system can work stable over long periods and the process is ready for full-scale implementation. Currently, an Anammox reactor is being built at the Rotterdam Sluisjesdijk plant.
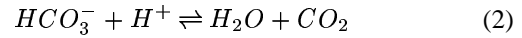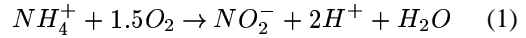
In this paper, the SHARON model is studied in view of coupling with the Anammox process. Special attention is given to the calculation of pH, as it is essential for future studies of the pH control, that is a key point in obtaining the desired ammonium/nitrite ratio. In this contribution, the behaviour of the SHARON reactor, operated without pH control, is presented.

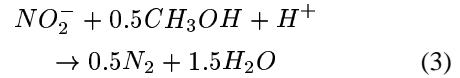## 2. PROCESS CONFIGURATION AND BASIC CONVERSION REACTIONS

The set-up of the SHARON process basically consists of a continuous, completely mixed reactor without sludge retention, operating at high temperature (35°C) and an average pH-value of about 7. Under these conditions, ammonium oxidizers grow faster than nitrite oxidizers, which can be washed out by sufficiently lowering the hydraulic retention time. The effluent ammonia concentration decreases with higher retention time, but is independent of the inlet ammonia concentration, a typical feature of a chemostat reactor. In this way, the SHARON process is better suited to achieve substantial ammonia conversion at high reaction rates for relatively concentrated flows, rather than to meet strict effluent standards. It is very well applicable for the treatment of reject water from sludge digestion, where high temperature and pH are taken advantage of.

For high-concentrated streams, the protons produced during nitrification would cause a significant pH drop, lowering the microbial conversion rates. In case the influent contains ammonium and bicarbonate on an equimolar basis, which can be reasonably assumed for

sludge digestion rejection water, half of the produced protons is removed via carbon dioxide stripping:

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + 2H^+ + H_2O \quad (1)$$
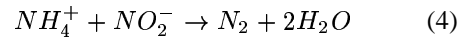$$HCO_3^- + H^+ \rightleftharpoons H_2O + CO_2 \quad (2)$$

However, as the reaction scheme above shows, this is not sufficient for pH control if nearly all ammonia has to be converted. The remaining half of the protons produced in reaction (1) can be consumed by denitrification of the produced nitrite. For this purpose, the reactor is cyclically aerated and during the anoxic phase a COD-source such as methanol is added:
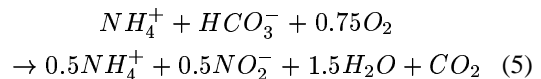
$$NO_2^- + 0.5CH_3OH + H^+$$
$$\rightarrow 0.5N_2 + 1.5H_2O \quad (3)$$

Denitrification for pH control by adding methanol is cheaper than alkali addition (Hellinga *et al.*, 1999). Note that denitrification is not an objective on its own, since the SHARON-effluent is usually recycled to the main wastewater treatment plant, where the remaining nitrite is converted.

The simplified Anammox reaction, neglecting biomass growth, can be written as

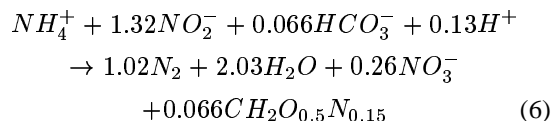$$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O \quad (4)$$

The required 1/1 ammonium/nitrite ratio for Anammox can be produced by operating the SHARON process without pH control, still assuming the SHARON influent contains equimolar amounts of ammonium and bicarbonate. Indeed, the moment half of the ammonium is converted to nitrite, the amount of protons produced is balanced by carbon dioxide stripping.

$$NH_4^+ + HCO_3^- + 0.75O_2$$
$$\rightarrow 0.5NH_4^+ + 0.5NO_2^- + 1.5H_2O + CO_2 \quad (5)$$

Further ammonia conversion than this 50% would lead to a pH drop, preventing further nitrification. In practice, the ammonium/nitrite ratio depends on the actual ammonium/bicarbonate ratio in the influent.

Besides, the optimal ammonium/nitrite influent ratio for the Anammox reactor, also requires further discussion, as the above mentioned 1/1 ratio has been derived for the simplified case in which biomass growth is not considered. Van Dongen *et al.* (2001b) assumed a biomass yield of 0.066, to come to the following overall Anammox reaction (including growth):

$$NH_4^+ + 1.32NO_2^- + 0.066HCO_3^- + 0.13H^+$$
$$\rightarrow 1.02N_2 + 2.03H_2O + 0.26NO_3^-$$
$$+0.066CH_2O_{0.5}N_{0.15} \quad (6)$$

In this case an ammonium/nitrite ratio of 1/1.32 would theoretically be optimal to feed the Anammox process. The ammonium/nitrite ratio needed in practice

depends on the actual growth yield. Note also that under the prevailing anoxic conditions of the Anammox process, a part of the produced nitrate can be heterotrophically denitrified to NO_2^-, again influencing the ammonium/nitrite ratio needed. In any case, process control is recommended to adjust the ammonium/nitrite ratio and in this way maximize the overall N-removal.

Experiments performed by van Dongen *et al.* (2001a) showed that the ammonium/nitrite ratio produced by the SHARON process can be sensitively influenced by changing the reactor pH between 6.5 and 7.5. On the one hand, as pH increases, the equilibrium between ammonia and ammonium shifts towards more ammonia. On the other hand, the concentration of ammonia, rather than ammonium being the actual substrate for nitrification, in a chemostat remains unchanged with changing pH. The combination of these two effects results in a lower ammonium effluent concentration with increasing pH. This control law can be used for setting the exact ratio for full nitrogen removal in the Anammox process. It is further studied how the existing model for the SHARON process with denitrification should be adapted for this purpose.

3. THE SHARON MODEL

To gain insight into the coupled SHARON-Anammox process, simulations have been performed using a Matlab-Simulink model. The reactor is of the CSTR type and consists of a liquid phase and a gas phase, both assumed to be perfectly mixed. Between these phases, transport of oxygen, carbon dioxide and nitrogen takes place.

3.1 *Liquid phase mass balances*

The liquid phase mass balance for a compound i with concentration C_i reads as

$$\frac{d(V_L \cdot C_{L,i})}{dt} = \Phi_L^{in} \cdot C_{L,i}^{in} - \Phi_L^{out} \cdot C_{L,i}$$
$$+ k_L a_i \cdot (C_{L,i}^* - C_{L,i}) \cdot V_L + r_i \cdot V_L \qquad (7)$$

The liquid phase volume V_L is assumed to be constant in comparison with liquid phase concentration changes. Liquid phase concentrations are calculated by integrating the corresponding mass balances. The components considered are given in Table 1.

3.2 *Biological conversion reactions*

Biological conversion reactions take place in the liquid phase only. Table 1 summarizes the stoichiometry of the processses considered in the form of the stoichiometric matrix (A_{ij}), expressed in terms of the corresponding yield coefficients and parameters indicating the biomass composition. All concentrations and reaction stoichiometries are expressed on a molar basis. Decay (or maintenance) is not included in the model, as it is assumed to have little impact in systems that operate at high microbial specific growth rates (Hellinga *et al.*, 1999).

The process rates ρ_j for each reaction j (expressed in mol m$_L^{-3}$ s^{-1}) are summarized in Table 2. The values of the kinetic parameters are given in the appendix. From these reaction rates, the volumetric conversion rate r_i of a component i is calculated as

$$r_i = \sum_{j=1}^{5} A_{ij} \cdot \rho_j \qquad (8)$$

Note that the conversion rate is negative for components that undergo net consumption. In contrast with the industry-standard Activated Sludge Models (Henze *et al.*, 2000), microbial reaction rates are expressed here as functions of the actual substrates, i.e. the charged or uncharged appearance of the compounds. This approach is preferred in order to cover the pH influence in a more straightforward manner.

3.3 *Calculation of pH and equilibrium concentrations*

The liquid phase concentrations of some of the components are related to each other by equilibrium reactions. Equilibria are considered for ammonia/ammonium, nitrous acid/nitrite, carbonate/bicarbonate/carbon dioxide and water. Lumped components are defined for which the concentrations equal the total concentration of the components, active in an equilibrium:

$$C_{TNH} = C_{NH_3} + C_{NH_4^+} \qquad (9)$$
$$C_{TNO} = C_{HNO_2} + C_{NO_2^-} \qquad (10)$$
$$C_{IC} = C_{CO_2} + C_{HCO_3^-} + C_{CO_3^{2-}} \qquad (11)$$

At each time step, the concentrations of the components that are not involved in a chemical equilibrium, are directly calculated by integrating the corresponding mass balance accumulation terms. The concentrations of the lumped components (9)-(11) are obtained by integrating the sum of the accumulation terms of the different forms corresponding to that equilibrium.

The necessity to calculate the concentration of the lumped components first instead of immediately calculating the concentrations of the individual components taking part in a chemical equilibrium, is in the first place due to the fact that every change in the concentration of a component involved in a chemical equilibrium, causes changes in the concentrations of all components taking part in that equilibrium.

Table 1. Stoichiometric matrix (A_{ij}) in terms of yield coefficients and biomass composition

A_{ij}	j process considered				
i component [mole m$_L^{-3}$]	1 ammonium oxidation	2 nitrite oxidation	3 denitrification nitrite	4 denitrification nitrate	5 methanol oxidation
1 protons	$\frac{2}{Y_1} - n_{amm}$	n_{nit}	$-\left(\frac{1}{Y_3} - n_{het}\right)$	$-\left(\frac{1}{Y_4} - n_{het}\right)$	n_{het}
2 nitrous acid	0	0	0	0	0
3 nitrite	$\frac{1}{Y_1} - n_{amm}$	$-\frac{1}{Y_2}$	$-\frac{1}{Y_3}$	0	0
4 nitrate	0	$\frac{1}{Y_2}$	0	$-\frac{1}{Y_4}$	0
5 ammonia	0	0	0	0	0
6 ammonium	$-\frac{1}{Y_1}$	$-n_{nit}$	$-n_{het}$	$-n_{het}$	$-n_{het}$
7 bicarbonate	0	0	0	0	0
8 carbonate	0	0	0	0	0
9 methanol	0	0	0	0	$-\frac{1}{Y_5}$
10 oxygen	$-\left(-1+\frac{1.5}{Y_1} - \frac{h_{amm}}{4} + \frac{o_{amm}}{2} - \frac{5}{4} * n_{amm}\right)$	$-\left(-1+\frac{0.5}{Y_2} - \frac{h_{nit}}{4} + \frac{o_{nit}}{2} + \frac{3}{4} * n_{nit}\right)$	$-\left(\frac{2}{3} + \frac{0.5}{Y_3} + \frac{h_{het}}{6} - \frac{o_{het}}{3} - \frac{n_{het}}{2}\right)$	$-\left(\frac{2}{3} + \frac{5}{6*Y_4} + \frac{h_{het}}{6} - \frac{o_{het}}{3} - \frac{n_{het}}{2}\right)$	$-\left(-1+\frac{1.5}{Y_5} - \frac{h_{het}}{4} + \frac{o_{het}}{2} + \frac{3}{4} * n_{het}\right)$
11 carbon dioxide	-1	-1	$-\frac{1}{3} + \frac{0.5}{Y_3} + \frac{h_{het}}{6} - \frac{n_{het}}{2} - \frac{o_{het}}{3}$	$-\left(-\frac{1}{3} + \frac{5}{6*Y_4} + \frac{h_{het}}{6} - \frac{n_{het}}{2} - \frac{o_{het}}{3}\right)$	$-1 + \frac{1}{Y_5}$
12 nitrogen	0	0	$\frac{0.5}{Y_3}$	$\frac{0.5}{Y_4}$	0
13 X_{amm}	1	0	0	0	0
14 X_{nit}	0	1	0	0	0
15 X_{het}	0	0	1	1	1
$Y_j \left[\frac{\text{mole X}}{\text{mole substrate}}\right]$	$0.11 \cdot \frac{14}{M_{amm}}$ [2]	$0.03 \cdot \frac{14}{M_{nit}}$ [2]	0.23 [1]	0.33 [1]	0.29 [1]
$CH_{h_i}O_{o_i}N_{n_i}$	$CH_{1.8}O_{0.5}N_{0.2}$	$CH_{1.8}O_{0.5}N_{0.2}$		$CH_{1.8}O_{0.5}N_{0.2}$	

(1) Value at 35°C, Lochtman (1995)
(2) Value at 35°C, Wiesmann (1994)

A second reason for calculating the concentration of lumped components first, lies in the formulation of the stoichiometric matrix. Although ammonia rather than ammonium and nitrous acid rather than the nitrite ion are the actual substrates for the nitrification processes (Anthonisen *et al.*, 1976), the stoichiometry of the reactions summarized in Table 1 is expressed in terms of ammonium and nitrite, as typically done. In the same way, the stoichiometric matrix doesn't contain coefficients for bicarbonate and carbonate, but only for carbon dioxide. The process rates given in Table 2 are expressed in terms of the real substrate. As the conversion rates are calculated from the process rates of Table 2 and the stoichiometric coefficients of Table 1 according to equation (8), they will only be correct for components that are not involved in chemical equilibria. The same will be valid for the accumulation terms in the mass balances (7), in which the conversion rates appear. For the components involved in a chemical equilibrium, only the sum of the accumulation terms of the different forms under which they occur, is corresponding to reality. This is corrected by considering lumped components first and subsequently calculating the concentrations of the individual components from the concentrations of the lumped components, the equilibrium constants and the pH, once the latter is known and before the next time step is initiated.

Although stoichiometric coefficients for protons are taken up in Table 1 for reasons of completeness, they are not actually implemented in the Matlab/Simulink model. On the contrary, the proton concentration in the reactor is calculated from the charge balance in the reactor, in order to assure the sum of all charges to be zero. The charge balance in the reactor can be written as

$$-C_{H+} + C_{OH-} - C_{NH_4^+} + C_{NO_2^-}$$
$$+C_{HCO_3^-} + 2C_{CO_3^{2-}} - C_{Z+} = \Delta_{ch} \quad (12)$$

in which Δ_{ch} stands for the 'gap' in the charge balance, which should theoretically be close to zero. The ions originating from strong acids or bases (e.g. Na^+, K^+, Cl^-, F^-), that are not influenced by the establishment of an equilibrium pH, are accounted for by a lumped, artifical component, Z^+. It represents the amount of net positive charges, expressed in mol m_L^{-3}. Note that this concentration is negative if there are more negative than positive charges present. As these net positive charges are not involved in any conversions considered, their concentration in the perfectly mixed reactor is only determined by the concentration entering the reactor and their initial concentration in the reactor. These concentrations can be calculated from the charge balances for the influent and for the initial concentrations respectively. Every time step, C_{Z+} is calculated from the corresponding mass balance.

Once C_{Z+} is known, the pH is calculated in the following way. As chemical equilibrium reactions proceed much faster than the biological conversion reactions, they are assumed to be in steady state, so the following equations apply:

$$Ke_{NH_4} = \frac{C_{NH_3} \cdot C_{H+}}{C_{NH_4^+}} \quad (13)$$

$$Ke_{HNO_2} = \frac{C_{H+} \cdot C_{NO_2^-}}{C_{HNO_2}} \quad (14)$$

$$Ke_{CO_2} = \frac{C_{H+} \cdot C_{HCO_3^-}}{C_{CO_2}} \quad (15)$$

$$Ke_{HCO_3} = \frac{C_{H+} \cdot C_{CO_3^{2-}}}{C_{HCO_3^-}} \quad (16)$$

$$K_W = C_{H+} \cdot C_{OH-} \quad (17)$$

By substituting the concentrations of the lumped components (9)-(11) into the steady state expressions for equilibria (13)-(17), the concentration of every charged component can be rewritten in terms of the concentration of protons and lumped components:

$$C_{NH_4^+} = \frac{C_{TNH}}{1 + \frac{Ke_{NH_4}}{C_{H+}}} \quad (18)$$

$$C_{NO_2^-} = \frac{C_{TNO}}{1 + \frac{C_{H+}}{Ke_{HNO_2}}} \quad (19)$$

$$C_{CO_3^{2-}} = \frac{C_{IC}}{\frac{C_{H+}^2}{Ke_{CO_2} \cdot Ke_{HCO_3}} + \frac{C_{H+}}{Ke_{HCO_3}} + 1} \quad (20)$$

$$C_{HCO_3^-} = \frac{C_{IC}}{\frac{C_{H+}}{Ke_{CO_2}} + 1 + \frac{Ke_{HCO_3}}{C_{H+}}} \quad (21)$$

The expressions (18)-(21) are substituted in the charge balance (12), in which the pH remains the only unknown:

$$\Delta_{ch}(C_{H+}) = -C_{H+} + \frac{K_W}{C_{H+}} - \frac{C_{TNH}}{1 + \frac{Ke_{NH_4}}{C_{H+}}}$$

$$+ \frac{C_{TNO}}{1 + \frac{C_{H+}}{Ke_{HNO_2}}} + \frac{C_{IC}}{\frac{C_{H+}}{Ke_{CO_2}} + 1 + \frac{Ke_{HCO_3}}{C_{H+}}}$$

$$+ 2 \cdot \frac{C_{IC}}{\frac{C_{H+}^2}{Ke_{CO_2} \cdot Ke_{HCO_3}} + \frac{C_{H+}}{Ke_{HCO_3}} + 1} - C_{Z+} \quad (22)$$

This equation can be solved iteratively for C_{H+}, e.g. according to the Newton-Raphson method, from an initial guess $C_{H+,0}$.

Once the pH is known besides the concentrations of the lumped components, the concentration of the individual components, involved in an equilibrium, is calculated from the expressions (18)-(21) and (9)-(11).

As stated, the above reasoning assumes the concentration of net positive charges not to vary with varying pH, assuming these net positive charges originate from

Table 2. Kinetic rate expressions

process rate equation ρ_j [mole m$_L^{-3}$ s^{-1}]
$\rho_1 = \mu_{max}^{amm} \cdot \dfrac{C_{NH_3}}{K_{NH_3}^{amm} + C_{NH_3}} \cdot \dfrac{C_{O_2}}{K_{O_2}^{amm} + C_{O_2}} \cdot \dfrac{K_{I,HNO_2}^{amm}}{K_{I,HNO_2}^{amm} + C_{HNO_2}} \cdot X^{amm}$
$\rho_2 = \mu_{max}^{nit} \cdot \dfrac{C_{HNO_2}}{K_{HNO_2}^{nit} + C_{HNO_2}} \cdot \dfrac{C_{O_2}}{K_{O_2}^{nit} + C_{O_2}} \cdot X^{nit}$
$\rho_3 = \mu_{max}^{dNO_2} \cdot \dfrac{C_{NO_2}}{K_{NO_2}^{dNO_2} + C_{NO_2}} \cdot \dfrac{C_{CH_3OH}}{K_{CH_3OH}^{het,an} + C_{CH_3OH}} \cdot \dfrac{K_{I,O_2}}{K_{I,O_2} + C_{O_2}} \cdot X^{het}$
$\rho_4 = \mu_{max}^{dNO_3} \cdot \dfrac{C_{NO_3}}{K_{NO_3}^{dNO_3} + C_{NO_3}} \cdot \dfrac{C_{CH_3OH}}{K_{CH_3OH}^{het,an} + C_{CH_3OH}} \cdot \dfrac{K_{I,O_2}}{K_{I,O_2} + C_{O_2}} \cdot X^{het}$
$\rho_5 = \mu_{max}^{met} \cdot \dfrac{C_{CH_3OH}}{K_{CH_3OH}^{het,ox} + C_{CH_3OH}} \cdot \dfrac{C_{O_2}}{K_{O_2}^{het} + C_{O_2}} \cdot X^{het}$

strong acids/bases. In reality, weak acids or bases e.g. H_2S, H_3PO_4 and volatile fatty acids could contribute to the concentration of these net positive charges. Also, the steady state assumption might not be appropriate for the bicarbonate/carbon dioxide equilibrium, being rather slow. These assumptions can explain possible differences in the pH calculated by the model from acid-base equilibria and the measured pH.

3.4 Gas phase

No reactions are assumed to take place in the gas phase. Gas phase mass balances for oxygen, carbon dioxide and nitrogen are considered. In analogy with the liquid phase mass balances (7), the gas phase mass balance for a compound i reads as

$$\frac{d\left(V_G \cdot C_{G,i}\right)}{dt} = \Phi_G^{in} \cdot C_{G,i}^{in} - \Phi_G^{out} \cdot C_{G,i}$$
$$-k_L a_i \cdot \left(C_{L,i}^* - C_{L,i}\right) \cdot V_L \qquad (23)$$

4. SIMULATION RESULTS

The behaviour of the SHARON reactor, operated without denitrification, has been simulated. Simulations were performed for an inlet flow of 600 m$_L^3$ h^{-1}, containing 70 mole m$_L^{-3}$ of ammonium and an equal amount of bicarbonate at pH 7. The hydraulic retention time, equal to the sludge retention time (SRT), was varied by varying the liquid phase volume. The reactor was continuously aerated, so no denitrification took place. Figure 1, 2 and 3 present the steady state results (obtained after 50 days of simulation) in function of the SRT. The concentration of ammonia and nitrite oxidizers is given in Figure 1. Ingrowth of ammonia oxidizers starts at an SRT of 0.5 days. In order to prevent ingrowth of nitrite oxidizers, the SRT should be kept below 1.5 days. This can also be concluded from the corresponding nitrate formation, shown in Figure 2.
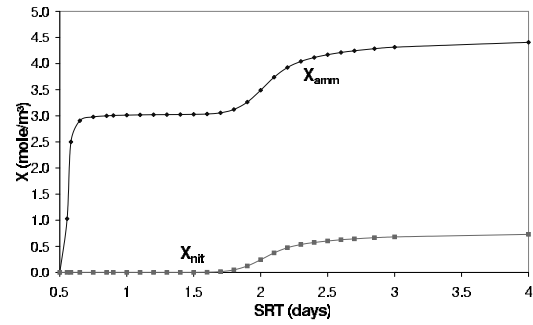

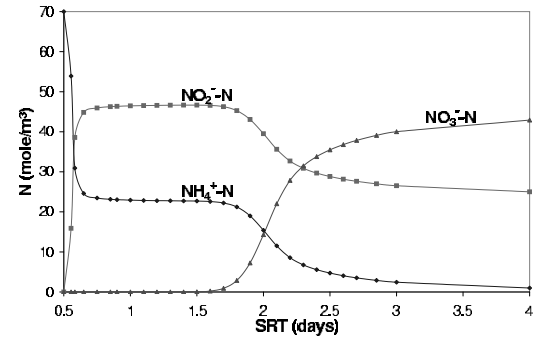Fig. 1. Influence of SRT on biomass concentrations

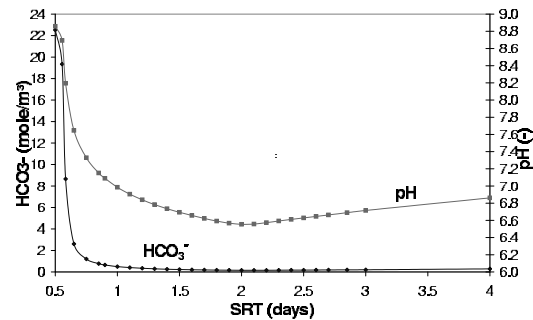Fig. 2. Influence of SRT on nitrogen compound concentrations

Fig. 3. Influence of SRT on pH and alkalinity

The optimal operating SRT could be chosen as 1 day, in order to keep a safety margin. At this retention time, total ammonium and nitrite are present in a ratio of about 2/1 at pH 7. Figure 3 shows that at this point, indeed almost all alkalinity is consumed. This value is quite different from the experimental result found by van Dongen et al. (2001a), who observed stable ammonium conversion without the formation of nitrate in a SHARON reactor without pH control (pH = 6.7 ± 0.3) to an ammonium/nitrite ratio of 1/1.13. This can probably be explained by deviations in the values of the model affinity constants from reality. Further study of the model parameters seems recommended.

5. CONCLUSION

Looking for sustainable N-removal techniques, this paper discusses the SHARON process for treating wastewater streams with high ammonia load, in view of its coupling with the Anammox process. For this purpose, a mathematical model of the SHARON process that takes into account pH effects was used. Preliminary simulations show that the ammonium/nitrite ratio, produced in the SHARON process without pH control, can deviate significantly from the desired 1/1 mixture. In future, pH control will be implemented in the model and its effect on the produced ammonium/nitrite ratio will be studied.

ACKNOWLEDGEMENT

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APPENDIX: GLOSSARY

symbol	characterization	dimension
A_{ij}	stoichiometric coefficient of component i in reaction j	mole
$C_{G,i}$	gas phase (bulk) concentration of component i	mole m_G^{-3}
$C_{G,i}^{in}$	inlet concentration of component i	mole m_G^{-3}
$C_{L,i}$	liquid phase (bulk) concentration of component i	mole m_L^{-3}
$C_{L,i}^{in}$	inlet concentration of component i	mole m_L^{-3}
$C_{L,i}^*$	saturation concentration of component i at gas/liquid interphase	mole m_L^{-3}
$k_L a_i$	volumetric mass transfer coefficient for component i	s^{-1}
M	molar mass	g mole^{-1}
r_j	volumetric conversion rate of reaction j	mole m_L^{-3} s^{-1}
R_i	volumetric production rate of component i	mole m_L^{-3} s^{-1}
V_G	gas phase volume	m_G^3
V_L	liquid phase volume	m_L^3
Y_j	yield coefficient for reaction j	mole X (mole substrate)$^{-1}$
Φ_G^{in}	inlet volumetric gas flow rate	m_G^3 s^{-1}
Φ_G^{out}	outlet volumetric gas flow rate	m_G^3 s^{-1}
$\Phi_{L,in}$	inlet volumetric flow rate	m_L^3 s^{-1}
$\Phi_{L,out}$	outlet volumetric flow rate	m_L^3 s^{-1}

symbol	characterization	dimension	value
	maximum specific growth rates		
μ_{max}^{amm}	ammonia oxidizers	s^{-1}	2.43E-5 [1]
μ_{max}^{nit}	nitrite oxidizers	s^{-1}	1.22E-5 [1]
$\mu_{max}^{dNO_2}$	nitrite denitrifiers	s^{-1}	1.74E-5 [1]
$\mu_{max}^{dNO_3}$	nitrate denitrifiers	s^{-1}	3.01E-5 [2]
μ_{max}^{met}	methanol oxidizers	s^{-1}	8.33E-5 [2]
	affinity constants		
$K_{NH_3}^{amm}$	ammonia (for ammonia oxidzers)	mole m_L^{-3}	0.0334 [1]
$K_{O_2}^{amm}$	oxygen (for ammonia oxidizers)	mole m_L^{-3}	0.045 [1]
$K_{HNO_2}^{nit}$	nitrous acid (for nitrite oxidizers)	mole m_L^{-3}	0.019 [2]
$K_{O_2}^{nit}$	oxygen (for nitrite oxidizers)	mole m_L^{-3}	0.034 [2]
$K_{NO_2}^{dNO_2}$	nitrite (for nitrite denitrifiers)	mole m_L^{-3}	0.0085 [2]
$K_{CH_3OH}^{het,an}$	methanol (during anoxic growth)	mole m_L^{-3}	0.521 [2]
$K_{NO_3}^{dNO_3}$	nitrate (for nitrate denitrifiers)	mole m_L^{-3}	0.01 [2]
$K_{CH_3OH}^{het,ox}$	methanol (during oxic growth)	mole m_L^{-3}	2.083 [2]
$K_{O_2}^{het}$	oxygen (for methanol oxidizers)	mole m_L^{-3}	0.0025 [2]
	inhibition constants		
K_{I,HNO_2}^{amm}	nitrous acid (for ammonia oxidizers)	mole m_L^{-3}	0.0145 [1]
K_{I,O_2}	'mathematical switch'	mole m_L^{-3}	0.0001
	equilibrium constants		
Ke_{NH_4}	ammonium equilibrium constant	mole m_L^{-3}	1.13E-6 [1]
Ke_{HNO_2}	nitrous acid equilibrium constant	mole m_L^{-3}	5.71E-1 [1]
Ke_{CO_2}	carbon dioxide equilibrium constant	mole m_L^{-3}	4.91E-4 [1]
Ke_{HCO_3}	bicarbonate equilibrium constant	mole m_L^{-3}	1.24E-6 [1]
K_W	water dissociation constant	mole^2 m_L^{-6}	1.89E-8 [1]

[1] Value at 35°C, Lochtman (1995)
[2] Value at 35°C, Wiesmann (1994)