

1 **Supplementary material: Analysing the effects of the aeration pattern and**
2 **residual ammonium concentration in a partial nitrification-anammox process**

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9 Temperature and pH effect on ionization constants

10 Eqs. (S1) and (S2), derived from acid-base equilibriums, were used for the calculation of the free
11 ammonia (FA or NH₃) and the free nitrous acid (FNA or HNO₂).

$$12 \quad FA = \frac{S_{NH_4} \cdot 10^{pH}}{\frac{K_b}{K_w} + 10^{pH}} \cdot \frac{14}{17} \quad (S1)$$

$$13 \quad FNA = \frac{S_{NO_2}}{K_a \cdot 10^{pH} + 1} \cdot \frac{47}{14} \quad (S2)$$

14 The ratio between the ionization constant of the ammonia equilibrium (K_b) and the ionization
15 constant of water (K_w) is related to the temperature as shown in Eq. (S3) and the temperature
16 effect on the ionization constant of the nitrous acid equilibrium (K_a) is shown in Eq. (S4)
17 (Anthonisen *et al.*, 1976).

$$18 \quad \frac{K_b}{K_w} = \exp\left(\frac{6344}{273+T}\right) \quad (S3)$$

$$19 \quad K_a = \exp\left(\frac{-2300}{273+T}\right) \quad (S4)$$

20 The kinetics for each of the processes considered i.e. growth and decay of each kind of bacteria
21 are shown in Table S2-Supplementary Material. In addition, the oxygen limitations, substrate
22 and non-competitive inhibitions for AOB and NOB growth processes were also considered.
23 AOB inhibition by FA and NOB inhibition by FNA were described with a Haldane model while
24 AOB inhibition by FNA and NOB inhibition by FA were described with a non-competitive
25 model.

Table S 1. Stoichiometric matrix (Mozumder et al., 2013).

component →	S _S	S _{NH4}	S _{NO2}	S _{NO3}	S _{O2}	S _{N2} [gN.m ⁻³]		X _{AOB}	X _{NOB}	X _{AMX}	X _{HET} [gCOD.m ⁻³]			X _I
	[gCOD. m ⁻³]	[gN.m ⁻³]	[gN.m ⁻³]	[gN.m ⁻³]	[gO ₂ .m ⁻³]	S _{N2AMX}	S _{N2H}	[gCOD. m ⁻³]	[gCOD. m ⁻³]	[gCOD. m ⁻³]	X _{O2,HET}	X _{NO2,HET}	X _{NO3,HET}	[gCOD. m ⁻³]
process ↓						[gN. m ⁻³]	[gN m ⁻³]				[gCOD. m ⁻³]	[gCOD. m ⁻³]	[gCOD. m ⁻³]	
<i>growth</i>														
1. growth of X _{AOB}		-1/Y _{AOB} - i _{NXB}	1/Y _{AOB}		1- 3.43/Y _{AOB}			1						
2. growth of X _{NOB}		-i _{NXB}	-1/Y _{NOB}	1/Y _{NOB}	1- 1.14/Y _{NOB}				1					
3. growth of anammox		-1/Y _{AMX} - i _{NXB}	-(1/Y _{AMX}) - (1/1.14)	1/1.14		2/ Y _{AMX}				1				
4. aerobic growth of heterotrophs	-1/Y _{HET}	-i _{NXB} + 1/Y _{HET} · i _{NSS}			1- 1/Y _{HET}						1			
5. anoxic (on NO ₂ ⁻) growth of heterotrophs	-1/ Y _{HET,NO2}	-i _{NXB} + 1/Y _{HET} · i _{NSS}	-(1-Y _{HET,NO2})/ (1.71Y _{HET,NO2})					(1-Y _{HET,NO2})/ (1.71Y _{HET,NO2})				1		
6. anoxic (on NO ₃ ⁻) growth of heterotrophs	-1/ Y _{HET,NO3}	-i _{NXB} + 1/Y _{HET} · i _{NSS}	(1-Y _{HET,NO3})/ (1.14Y _{HET,NO3})	-(1-Y _{HET,NO3})/ (1.14Y _{HET,NO3})										1
<i>decay</i>														
7. decay of X _{AOB}	1-f _I	i _{NXB} - f _I i _{NXI} - (1-f _I) i _{NSS}						-1						f _I
8. decay of X _{NOB}	1-f _I	i _{NXB} - f _I i _{NXI} - (1-f _I) i _{NSS}							-1					f _I
9. decay of X _{AMX}	1-f _I	i _{NXB} - f _I i _{NXI} - (1-f _I) i _{NSS}								-1				f _I
10. decay of X _{HET}	1-f _I	i _{NXB} - f _I i _{NXI} - (1-f _I) i _{NSS}										-1		f _I

Table S2. Kinetic rate expressions.

j	Process	Process rate (d ⁻¹)	Reference
1	Growth of X _{AOB}	$\mu_{\max, AOB} \cdot \frac{S_{O_2}}{K_{O_2, AOB} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{S, NH_4, AOB} + S_{NH_4} + \frac{S_{NH_4}^2}{K_{I, NH_4, AOB}}} \cdot \frac{K_{I, NO_2, AOB}}{K_{I, NO_2, AOB} + S_{NO_2}} \cdot X_{AOB}$	(Jubany <i>et al.</i> , 2008)
2	Decay of X _{AOB}	$b_{AOB} \cdot X_{AOB}$	(Volcke <i>et al.</i> , 2010)
3	Growth of X _{NOB}	$\mu_{\max, NOB} \cdot \frac{S_{O_2}}{K_{O_2, NOB} + S_{O_2}} \cdot \frac{S_{NO_2}}{K_{S, NO_2, NOB} + S_{NO_2} + \frac{S_{NO_2}^2}{K_{I, NO_2, NOB}}} \cdot \frac{K_{I, NH_4, NOB}}{K_{I, NH_4, NOB} + S_{NH_4}} \cdot X_{NOB}$	(Jubany <i>et al.</i> , 2008)
4	Decay of X _{NOB}	$b_{NOB} \cdot X_{NOB}$	(Volcke <i>et al.</i> , 2010)
5	Growth of X _{AMX}	$\mu_{\max, AMX} \cdot \frac{K_{I, O_2, AMX}}{K_{I, O_2, AMX} + S_{O_2}} \cdot \frac{S_{NH_4}}{K_{NH_4, AMX} + S_{NH_4}} \cdot \frac{S_{NO_2}}{K_{NO_2, AMX} + S_{NO_2}} \cdot X_{AMX}$	(Volcke <i>et al.</i> , 2010)
6	Decay of X _{AMX}	$b_{AMX} \cdot X_{AMX}$	(Volcke <i>et al.</i> , 2010)
7	Growth of X _{O2,HET}	$\mu_{\max, HET} \cdot \frac{S_{O_2}}{K_{O_2, HET} + S_{O_2}} \cdot \frac{S_S}{K_{S, HET} + S_S} \cdot \frac{S_{NH_4}}{K_{NH_4, HET} + S_{NH_4}} \cdot X_{HET}$	(Volcke <i>et al.</i> , 2010)
8	Growth of X _{NO2,HET}	$\mu_{\max, HET} \cdot \eta_{NO_2} \cdot \frac{K_{O_2, HET}}{K_{O_2, HET} + S_{O_2}} \cdot \frac{S_{NO_2}}{K_{NO_2, HET} + S_{NO_2}} \cdot \frac{S_S}{K_{S, HET} + S_S} \cdot \frac{S_{NO_2}}{S_{NO_2} + S_{NO_3}} \cdot \frac{S_{NH_4}}{K_{NH_4, HET} + S_{NH_4}} \cdot X_{HET}$	(Volcke <i>et al.</i> , 2010)
9	Growth of X _{NO3,HET}	$\mu_{\max, HET} \cdot \eta_{NO_3} \cdot \frac{K_{O_2, HET}}{K_{O_2, HET} + S_{O_2}} \cdot \frac{S_{NO_3}}{K_{NO_3, HET} + S_{NO_3}} \cdot \frac{S_S}{K_{S, HET} + S_S} \cdot \frac{S_{NO_3}}{S_{NO_2} + S_{NO_3}} \cdot \frac{S_{NH_4}}{K_{NH_4, HET} + S_{NH_4}} \cdot X_{HET}$	(Volcke <i>et al.</i> , 2010)
10	Decay of X _{HET}	$b_{HET} \cdot X_{HET}$	(Volcke <i>et al.</i> , 2010)

Table S3. Stoichiometric and kinetics parameters values

parameter	value	Unit	
Stoichiometric parameters			
Y_{AOB}	0.20	g COD.g ⁻¹ N	(Wiesmann, 1994) ⁽¹⁾
Y_{NOB}	0.057	g COD.g ⁻¹ N	(Wiesmann, 1994) ⁽¹⁾
Y_{AMX}	0.17	g COD.g ⁻¹ N	(Strous <i>et al.</i> , 1998) ⁽²⁾
Y_{HET}	0.67	g COD.g ⁻¹ COD	(Henze <i>et al.</i> , 2000)
$Y_{HET,NO2}$	0.53	g COD.g ⁻¹ COD	(Muller <i>et al.</i> , 2003)
$Y_{HET,NO3}$	0.53	g COD.g ⁻¹ COD	(Muller <i>et al.</i> , 2003)
i_{NXB}	0.07	g N.g ⁻¹ COD	(Mozumder <i>et al.</i> , 2013)
i_{NXI}	0.07	g N.g ⁻¹ COD	(Mozumder <i>et al.</i> , 2013)
i_{NSS}	0.03	g N.g ⁻¹ COD	(Henze <i>et al.</i> , 2000)
f_I	0.08	g COD.g ⁻¹ COD	(Henze <i>et al.</i> , 2000)
Kinetic parameters (at 30°C & pH 7)			
$\mu_{max,AOB}$	1.36	d ⁻¹	(Hellinga <i>et al.</i> , 1999) ⁽³⁾
$\mu_{max,NOB}$	0.79	d ⁻¹	(Hellinga <i>et al.</i> , 1999) ⁽³⁾
$\mu_{max,AMX}$	0.052	d ⁻¹	(Strous <i>et al.</i> , 1998) ⁽³⁾
$\mu_{max,HET}$	12	d ⁻¹	(Henze <i>et al.</i> , 2000) ⁽⁴⁾
$K_{S,NH4,AOB}$	1.1	g N.m ⁻³	(Wiesmann, 1994) ⁽⁵⁾
$K_{S,NO2,NOB}$	0.51	g N.m ⁻³	(Wiesmann, 1994) ⁽⁵⁾
$K_{NH4,AMX}$	0.03	g N.m ⁻³	Assumed, such that ratio $K_{NH}^{AOB} : K_{NH}^{AN}$ is about the same as in Hao <i>et al.</i> , (2002)

$K_{NO_2,AMX}$	0.005	g N.m^{-3}	Assumed, such that ratio $K_{NO_2}^{NOB} : K_{NO_2}^{AN}$ is about the same as in Hao <i>et al.</i> , (2002)
$K_{NO_2,HET}$	0.3	g N.m^{-3}	(Alpkvist <i>et al.</i> , 2006)
$K_{NO_3,HET}$	0.3	g N.m^{-3}	(Alpkvist <i>et al.</i> , 2006)
$K_{S,HET}$	20	g COD.m^{-3}	(Henze <i>et al.</i> , 2000)
$K_{O_2,AOB}$	0.3	$\text{g O}_2.\text{m}^{-3}$	(Wiesmann, 1994)
$K_{O_2,NOB}$	1.1	$\text{g O}_2.\text{m}^{-3}$	(Wiesmann, 1994)
$K_{I,O_2,AMX}$	0.05	$\text{g O}_2.\text{m}^{-3}$	(Mozumder <i>et al.</i> , 2013)
$K_{O_2,HET}$	0.2	$\text{g O}_2.\text{m}^{-3}$	(Henze <i>et al.</i> , 2000)
$K_{NH_4,HET}$	0.02	g N.m^{-3}	(Mozumder <i>et al.</i> , 2013)
$K_{I,NO_2,AOB}$	828	g N.m^{-3}	(Jubany <i>et al.</i> , 2009)
$K_{I,NH_4,AOB}$	9563	$\text{g N}^2.\text{m}^{-6}$	(Jubany <i>et al.</i> , 2009)
$K_{I,NH_4,NOB}$	154	g N.m^{-3}	(Jubany <i>et al.</i> , 2009)
$K_{I,NO_2,NOB}$	90	$\text{g N}^2.\text{m}^{-6}$	(Brockmann & Morgenroth, 2010)
b_{AOB}	0.068	d^{-1}	Assumed, set such that $b^{AOB} : \mu_{max}^{AOB} = b^H : \mu_{max}^H$
b_{NOB}	0.04	d^{-1}	Assumed, set such that $b^{NOB} : \mu_{max}^{NOB} = b^H : \mu_{max}^H$
b_{AMX}	0.0026	d^{-1}	Assumed, set such that $b^{AN} : \mu_{max}^{AN} = b^H : \mu_{max}^H$
b_{HET}	0.6	d^{-1}	Assumed $\mu_{max}^H / 20$ for this study

$\eta_{NO_2} = \eta_{NO_3}$	0.8	-	(Henze <i>et al.</i> , 2000)
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Mass transfer parameters

D_{NH_4}	1.5×10^{-4}	$m^2 \cdot d^{-1}$	(Williamson & McCarty, 1976)
D_{NO_2}	1.4×10^{-4}	$m^2 \cdot d^{-1}$	(Williamson & McCarty, 1976)
D_{NO_3}	1.4×10^{-4}	$m^2 \cdot d^{-1}$	(Williamson & McCarty, 1976)
D_{O_2}	2.2×10^{-4}	$m^2 \cdot d^{-1}$	(Picioreanu <i>et al.</i> , 1997)
D_S	1×10^{-4}	$m^2 \cdot d^{-1}$	(Hao & van Loosdrecht, 2004)

- (1) After unit conversion, using a typical biomass composition of $CH_{1.8}O_{0.5}N_{0.2}$, corresponding with $1.3659 \text{ g COD} \cdot \text{g}^{-1}$
- (2) After unit conversion, using a anammox biomass composition of $CH_2O_{0.5}N_{0.15}$, corresponding with $36.4 \text{ g COD} \cdot \text{mole}^{-1}$ or $1.51 \text{ g COD} \cdot \text{g}^{-1}$
- (3) Conversion of values given by Hellinga *et al.* (1999) at 35°C and by Strous *et al.* (1998) at 32.5°C to 30°C using the relationship (written for X_{AOB} , analogous for X_{NOB} and X_{AMX})

$$\mu_{max}^{AOB1}(T) = \mu_{max}^{AOB1}(T_{ref}) \cdot \exp\left(\frac{E_a^{AOB} \cdot (T - T_{ref})}{R \cdot T \cdot T_{ref}}\right)$$

with $E_a^{AOB} = 68 \text{ kJ} \cdot \text{mole}^{-1}$; $E_a^{NOB} = 44 \text{ kJ} \cdot \text{mole}^{-1}$; $E_a^{AMX} = 70 \text{ kJ} \cdot \text{mole}^{-1}$; $R = 8.31 \text{ J} \cdot \text{mole}^{-1} \cdot \text{K}^{-1}$.

- (4) Conversion of ASM1-values given by Henze *et al.* (2000), at 10°C and 20°C to 30°C using temperature relationship proposed by these authors (ASM3).
- (5) Calculated value at $T=30^\circ\text{C}$ and $\text{pH}=7$ from $K_{NH_3}^{AOB} = 0.028 \text{ g NH}_3\text{-N} \cdot \text{m}^{-3}$ and from $K_{HNO_2}^{NOB} = 3.2 \times 10^{-5} \text{ g HNO}_2\text{-N} \cdot \text{m}^{-3}$ considering the T and pH dependency of the chemical equilibrium $NH_4^+ \leftrightarrow NH_3 + H^+$ and $HNO_2 \leftrightarrow NO_2^- + H^+$

Table S4. References from the oxygen affinity values used in the study of NOB repression. $R_{KO} = K_{O_2, AOB} / K_{O_2, NOB}$.

$K_{O_2, AOB}$ (gO_2/m^3)	$K_{O_2, NOB}$ (gO_2/m^3)	R_{KO} ($K_{O_2, AOB} / K_{O_2, NOB}$)
0.3 (Wiesmann, 1994)	1.75 (Guisasola <i>et al.</i> , 2005)	0.17
0.3 (Wiesmann, 1994)	1.1 (Wiesmann, 1994)	0.27
0.16 (This study)	0.16 (Regmi <i>et al.</i> , 2014)	1
0.18 (Manser <i>et al.</i> , 2005)	0.13 (Manser <i>et al.</i> , 2005)	1.38
1.16 (Regmi <i>et al.</i> , 2014)	0.16 (Regmi <i>et al.</i> , 2014)	7.25

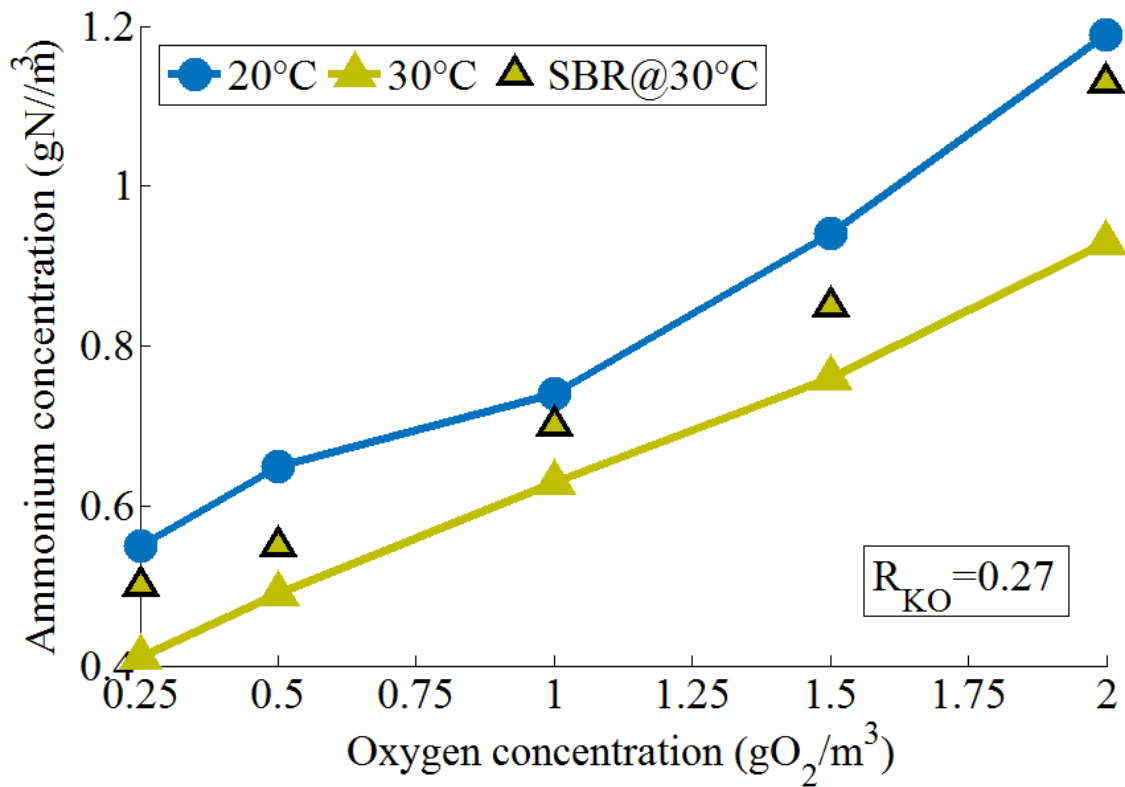


Figure S1. Comparison of the minimum ammonium concentrations for NOB repression obtained with a CSTR (label: 20°C and 30°C) and a SBR at 30°C (label: SBR 30°C). The values were obtained with an $R_{KO}=0.27$. It was observed that the values differ in average 13% and no more than 20%.

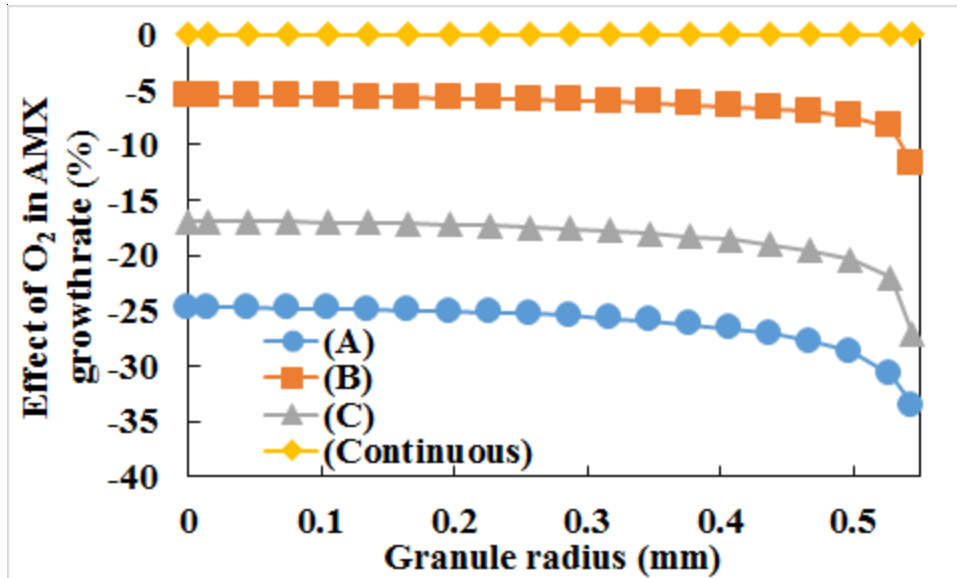


Figure S2. Reduction of anammox growth rate over the granule radius due to inhibition by oxygen in different aeration cases. The oxygen inhibition term $I_{O_2}(t, x) = K_{I, O_2, AMX} / (K_{I, O_2, AMX} + S_{O_2})$ averaged in time over the aeration period for each aeration case (A, B and C) was related to the one calculated for continuous aeration.

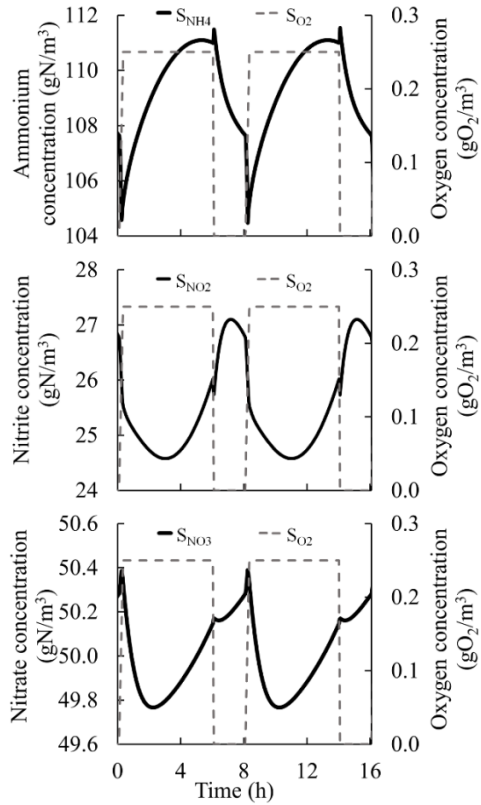


Figure S3. Concentrations in the bulk liquid during two cycles at steady state. The time axis represents the cycle time, not the total time since reactor start up. The dissolved oxygen was 0.25 g/m³ for the six-hour period of simultaneous feeding and continuous aeration, and then no aeration for the last two hours of the cycle. The temperature was 30°C, pH 7 and the granule diameter 1.1 mm.

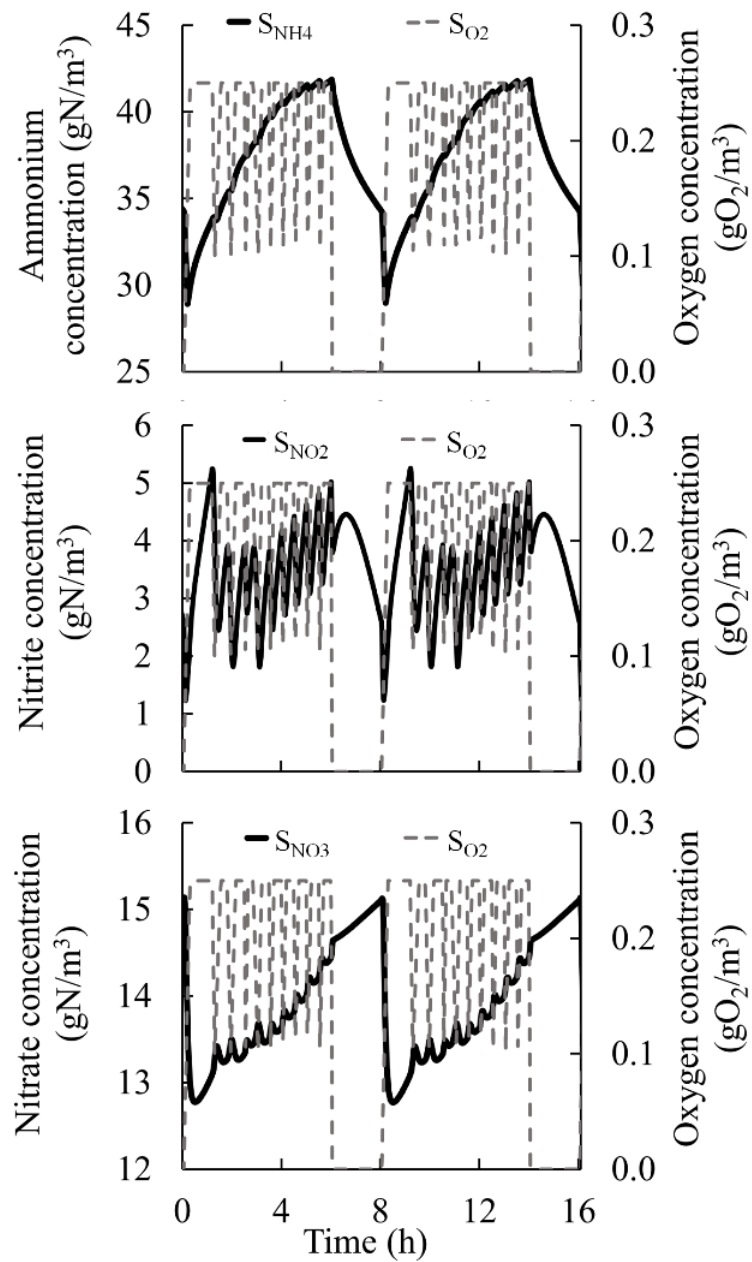


Figure S4. Concentrations during two cycles at steady state regarding bulk concentrations. Same operation parameters as in the multispecies granular sludge case except for the intermittent aeration.

References (Supplementary material)

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