Comparison of the Efficiency of Deammonification under Different DO concentration in a Laboratory-Scale Sequencing Batch Reactor

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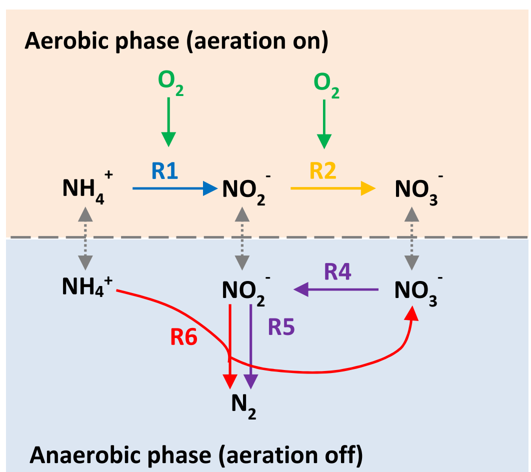

Figure S1. The conceptual model for nitrogen transformation under aeration on/off conditions. (R1: Aerobic growth of AOB; R2: Aerobic growth of NOB; R4-5: Anoxic growth of HDB; R6: Anaerobic growth of AnAOB).

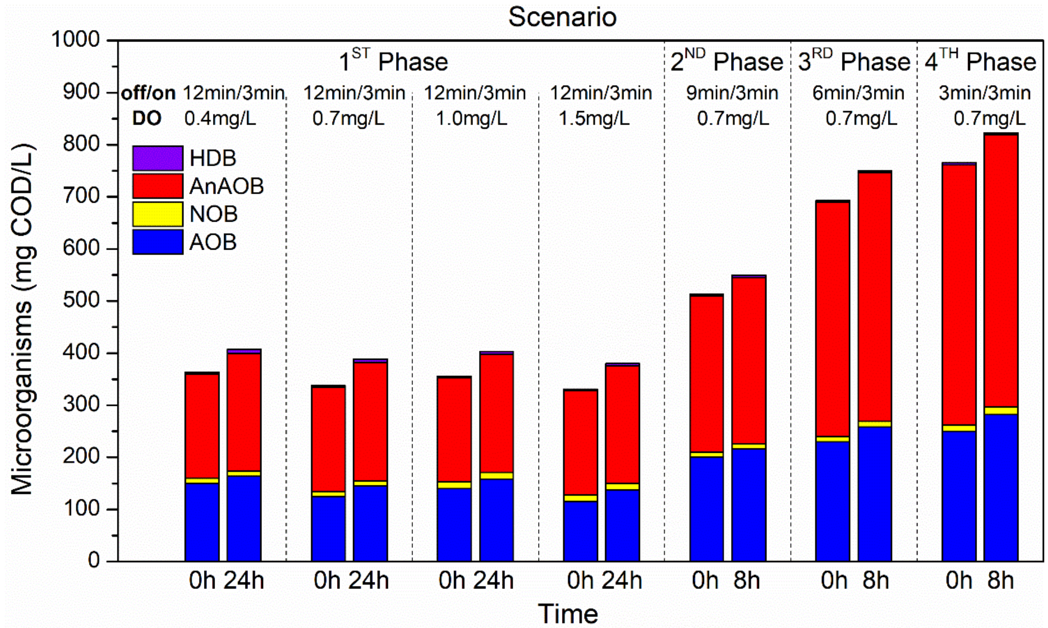

Figure S2. The initial microorganisms' composition and their predicted value after the batch test under different scenarios. (The initial composition was firstly estimated considering the results of our previous study (Al-Hazmi et al., 2020), metagenomic analysis and the measured MLVSS, and then the composition was slightly adjusted in during the preliminary model simulations).

Reference:

Al-Hazmi, H. E., Lu, X., Majtacz, J., et al. Optimization of the Aeration Strategies in a Deammonification Sequencing Batch Reactor for Efficient Nitrogen Removal and Mitigation of N_2O Production[J]. *Environmental Science & Technology*, **2020**, *55(2)*: 1218-1230.

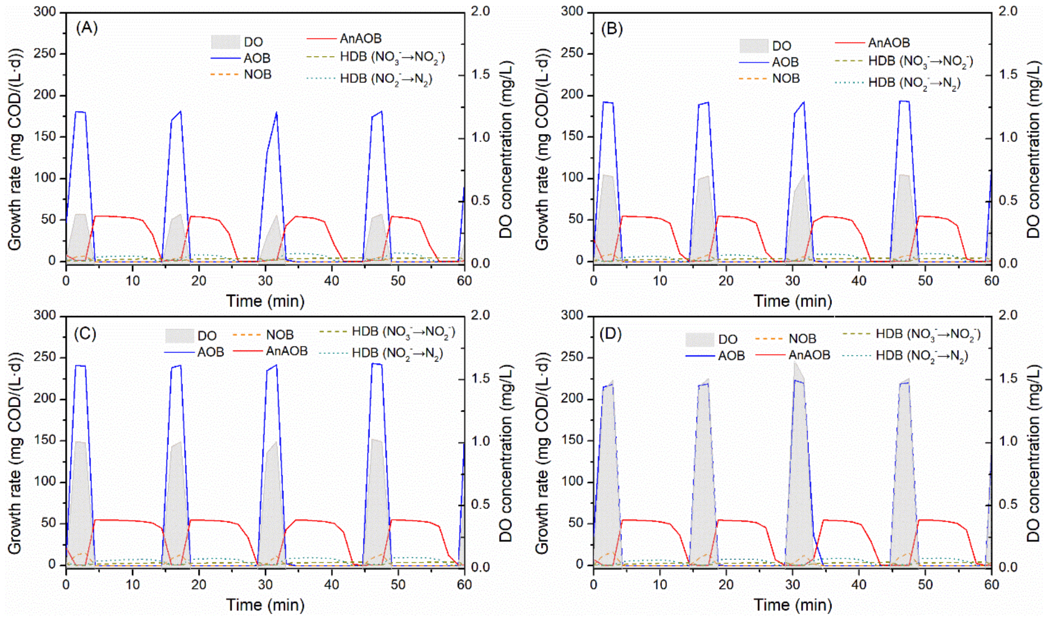

Figure S3. The variation in the simulated growth rates of different microorganisms with different DO set point of A) 0.4 mg O_2/L, B) 0.7 mg O_2/L, C) 1.0 mg O_2/L, D) 1.5 mg O_2/L at the same intermittent aeration mode off/on (12/3 min) conditions.

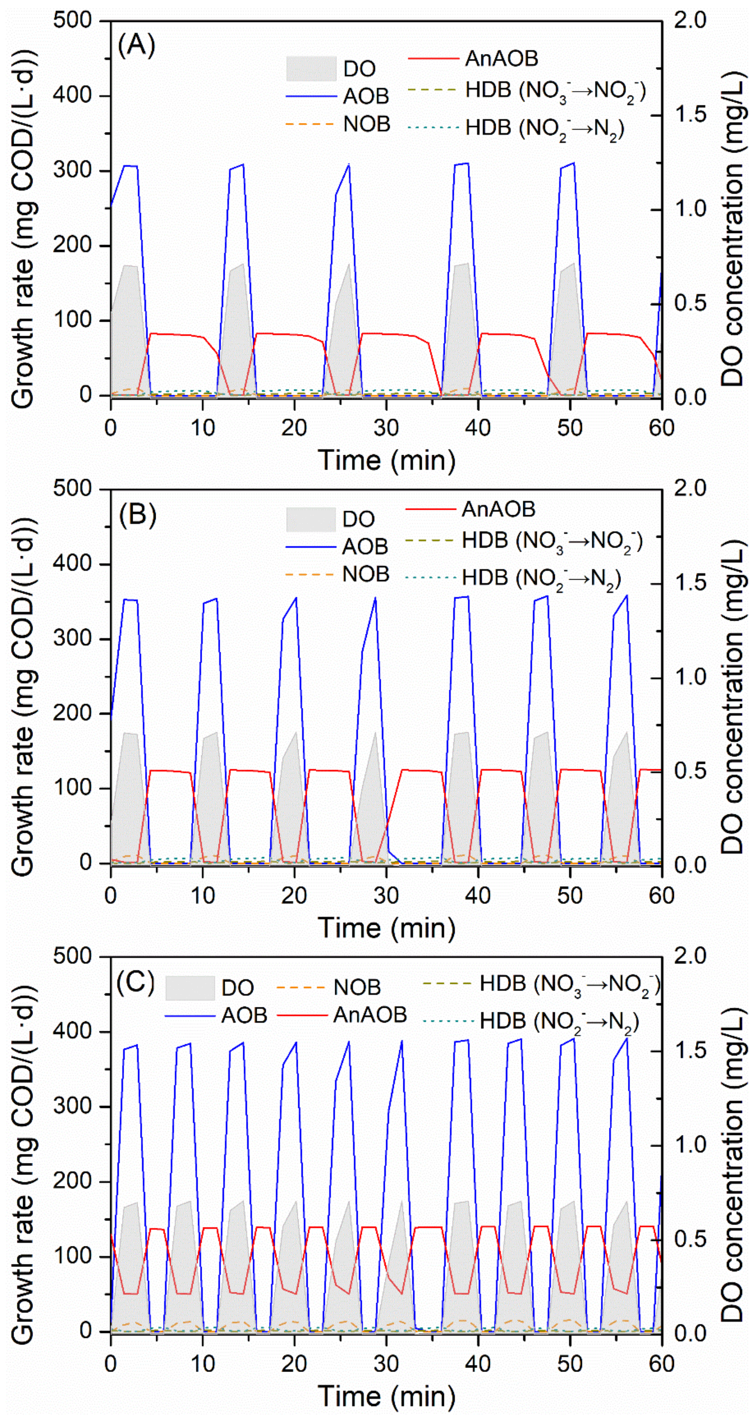

Figure S4. The variation in the simulated growth rates of different microorganisms with different intermittent aeration mode off/on A) 9min/3min, B) 6min/3min, C) 3min/3 min) at the same DO set point 0.7 mg O_2/L.

Table S1. Definition of the state variables of the proposed model.

No.	Symbol	State variable	Unit
1	S_I	Inert soluble matter	mg COD/L
2	S_S	Readily biodegradable substrate	mg COD/L
3	S_{O_2}	Dissolved oxygen	mg O_2/L
4	$S_{NO_3^-}$	Nitrate	mg N/L
5	$S_{NO_2^-}$	Nitrite	mg N/L
6	S_{N_2}	Nitrogen gas	mg N/L
7	$S_{NH_4^+}$	Ammonium and free ammonia	mg N/L
8	S_{ND}	Soluble biodegradable organic nitrogen	mg N/L
9	X_{AOB}	Aerobic ammonium-oxidizing biomass(AOB)	mg COD/L
10	X_{NOB}	Nitrite-oxidizing biomass(NOB)	mg COD/L
11	X_H	Aerobic heterotrophs biomass	mg COD/L
12	X_{HDB}	Anoxic heterotrophic denitrifying biomass (HDB)	mg COD/L
13	$X_{\mathrm{An}AOB}$	Anaerobic ammonium-oxidizing biomass (AnAOB)	mg COD/L
14	X_S	Slowly biodegradable substrate	mg COD/L
15	X_P	Particulate unbiodegradable matter	mg COD/L
16	X_{ND}	Particulate biodegradable organic nitrogen	mg N/L

Table S2. The matrix of the proposed model.

Component →i		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Process ↓ j		S_I	S_S	S_{O_2}	$S_{NO_3^-}$	$S_{NO_2^-}$	S_{N_2}	$S_{NH_4^+}$	S_{ND}	X_{AOB}	X_{NOB}	X_H	X_{HDB}	X_{AnAOB}	X_S	X_P	X_{ND}
R1	Aerobic growth of AOB, $NH_4^+ \rightarrow NO_2^-$			$-\frac{3.43-Y_{AOB}}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$		$-i_{XB}-\frac{1}{Y_{AOB}}$		1							
R2	Aerobic growth of NOB, $NO_2^- \rightarrow NO_3^-$			$-\frac{1.14-Y_{NOB}}{Y_{NOB}}$	$\frac{1}{Y_{NOB}}$	$-\frac{1}{Y_{NOB}}$		$-i_{XB}$			1						
R3	Aerobic growth of Heterotrophs		$-\frac{1}{Y_H}$	$-\frac{1-Y_H}{Y_H}$				$-i_{XB}$				1					
R4	Anoxic growth of HDB, $NO_3^- \rightarrow NO_2^-$		$-\frac{1}{Y_{HDB}}$		$-\frac{1-Y_{HDB}}{1.14Y_{HDB}}$	$\frac{1-Y_{HDB}}{1.14Y_{HDB}}$		$-i_{XB}$					1				
R5	Anoxic growth of HDB, $NO_2^- \rightarrow N_2$		$-\frac{1}{Y_{HDB}}$			$-\frac{1-Y_{HDB}}{1.71Y_{HDB}}$	$\frac{1-Y_{HDB}}{1.71Y_{HDB}}$	$-i_{XB}$					1				
R6	Anaerobic growth of AnAOB, $NH_4^+ + NO_2^- \rightarrow N_2 + NO_3^-$				$\frac{1}{1.41}$	$-\frac{1}{Y_{AnAOB}}-1.41$	$\frac{2}{Y_{AnAOB}}$	$-i_{XB}-\frac{1}{Y_{AnAOB}}$						1			
R7	Decay of AOB									-1					$1-f_P$	f_P	$i_{XB}-f_P i_{XP}$
R8	Decay of NOB										-1				$1-f_P$	f_P	$i_{XB}-f_P i_{XP}$
R9	Decay of Heterotrophs											-1			$1-f_P$	f_P	$i_{XB}-f_P i_{XP}$
R10	Decay of HDB												-1		$1-f_P$	f_P	$i_{XB}-f_P i_{XP}$
R11	Decay of AnAOB													-1	$1-f_P$	f_P	$i_{XB}-f_P i_{XP}$
R12	Hydrolysis of entrapped organics	f_I	$1-f_I$					i_{XS}							-1		
R13	Hydrolysis of entrapped organic N								1								-1
R14	Ammonification of soluble organic N							1	-1								

Table S3. The Kinetic equations of the proposed model.

Process ↓ j		Rate equation
R1	Aerobic growth of AOB, $NH_4^+ \rightarrow NO_2^-$	$\mu_{AOB}^{R1}\frac{S_{NH_4^+}}{K_{NH_4^+}^{R1}+S_{NH_4^+}}\frac{S_{O_2}}{K_{O_2}^{R1}+S_{O_2}}X_{AOB}$
R2	Aerobic growth of NOB, $NO_2^- \rightarrow NO_3^-$	$\mu_{NOB}^{R2}\frac{S_{NO_2^-}}{K_{NO_2^-}^{R2}+S_{NO_2^-}}\frac{S_{O_2}}{K_{O_2}^{R2}+S_{O_2}}X_{NOB}$
R3	Aerobic growth of Heterotrophs	$\mu_{H}^{R3}\frac{S_S}{K_S^{R3}+S_S}\frac{S_{O_2}}{K_{O_2,H}+S_{O_2}}X_H$
R4	Anoxic growth of HDB, $NO_3^- \rightarrow NO_2^-$	$\mu_{HDB}^{R4}\frac{S_S}{K_S^{R4}+S_S}\frac{S_{NO_3^-}}{K_{NO_3^-}^{R4}+S_{NO_3^-}}\frac{K_{i,O_2,HDB}}{K_{i,O_2,HDB}+S_{O_2}}\eta_g^{R4}X_{HDB}$
R5	Anoxic growth of HDB, $NO_2^- \rightarrow N_2$	$\mu_{HDB}^{R5}\frac{S_S}{K_S^{R5}+S_S}\frac{S_{NO_2^-}}{K_{NO_2^-}^{R5}+S_{NO_2^-}}\frac{K_{i,O_2,HDB}}{K_{i,O_2,HDB}+S_{O_2}}\eta_g^{R5}X_{HDB}$
R6	Anaerobic growth of AnAOB, $NH_4^+ + NO_2^- \rightarrow N_2 + NO_3^-$	$\mu_{AnAOB}^{R6}\frac{S_{NH_4^+}}{K_{NH_4^+}^{R6}+S_{NH_4^+}}\frac{S_{NO_2^-}}{K_{NO_2^-}^{R6}+S_{NO_2^-}}\frac{K_{i,O,AnAOB}}{K_{i,O,AnAOB}+S_{O_2}}X_{AnAOB}$
R7	Decay of AOB	$b_{AOB}X_{AOB}$
R8	Decay of NOB	$b_{NOB}X_{NOB}$

R9	Decay of Heterotrophs	$b_H X_H$
R10	Decay of HDB	$b_{HDB} X_{HDB}$
R11	Decay of AnAOB	$b_{AnAOB} X_{AnAOB}$
R12	Hydrolysis of entrapped organics	$k_h \frac{X_S/X_H}{K_X+(X_S/X_H)}\left[\left(\frac{S_{O_2}}{K_{O_2,H}+S_{O_2}}\right)+\eta_{hANOX}\left(\frac{K_{O_2,H}}{K_{O_2,H}+S_{O_2}}\right)\left(\frac{S_{NO_3^-}}{K_{NO_3^-}+S_{NO_3^-}}\right)\right]X_H$
R13	Hydrolysis of entrapped organic N	$r_{12}(X_{ND}/X_S)$
R14	Ammonification of soluble organic N	$K_a \cdot S_{ND} \cdot X_H$

Table S4. Stoichiometric parameters and conversion factors.

Symbol	Definition	Unit	Reference range	Default	Calibrated	References
Model stoichiometry						
Y_{AOB}	AOB yield	g COD/g N	0.15-0.24	0.18		1-13
Y_{NOB}	NOB yield	g COD/g N	0.041-0.06	0.06		1,3,5,6,7, 8,13,15
Y_{H}	heterotrophic yield	g COD/g COD	0.5-0.67	0.666		1,3,7,8,13, 14,16,17
Y_{HDB}	HDB yield	g COD/g COD	0.5-0.67	0.666		1,3,7,8,13, 14,16,17
Y_{AnAOB}	AMX yield	g COD/g N	0.114-0.17	0.17		13,15, 18-24
f_{P}	fraction of biomass leading to particulate products	g COD/g COD	0.08-0.2	0.08		1,3,7,13, 14,22
f_{I}	Production of soluble inerts in hydrolysis	g COD/g COD	0.02	0.02		14
Composite variable stoichiometry						
icv	XCOD/VSS	g COD/g VSS	1.42-1.48	1.48		14,25
fbod	BOD_5/BODultimate ratio	-	0.66	0.66		14
i_{XB}	N content of active biomass	g N/g COD	0.07-0.875	0.086		1-4,6-15, 18
i_{XP}	N content of endogenous/inert mass	g N/g COD	0.02-0.068	0.06		1,3,13,14
i_{XS}	nitrogen content of COD in slowly biodegradable substrate	g N/g COD	0.015	0.015		14

References: [1](Hiatt and Grady, 2008); [2](Law et al., 2012); [3](Ni et al., 2011); [4](Mampaey et al., 2011); [5](Wiesmann et al., 1994); [6](Mampaey et al., 2013); [7](Kampschreur et al., 2007); [8](Ni et al., 2013a); [9](Ni et al., 2013b); [10](Peng et al., 2015a and 2015b); [11](Pocquet et al., 2013); [12](Guo and Vanrolleghem, 2014); [13](von Schulthess and Gujer, 1996); [14](Henze et al., 2000); [15](Volcke et al., 2010); [16](Samie et al., 2011); [17](Pan et al., 2013); [18](Takács et al., 2007); [19](Koch et al., 2000); [20](Strous et al., 1998); [21](Bi et al., 2015); [22](Dapena-Mora et al., 2004); [23](Hao et al., 2002); [24](Ni et al., 2009); [25](Comeau, 2008)

Table S5. Kinetic parameters and their values (*value at T = 20°C).

Symbol	Definition	Unit	Reference range	Default	Calibrated	References
AOB						
μ_{AOB}^{R1}	the maximum specific growth rate	1/d	0.39-5.76	1.2		1-17
$K_{NH_4^+}^{R1}$	ammonia half saturation coefficient	g N/m^3	0.02-27.5	1		1,4,5, 8-12, 18-22
$K_{O_2}^{R1}$	oxygen half saturation coefficient	g O_2/m^3	0.02-2.1	0.4		1,2,4-6, 8-15, 18-20, 22,23
b_{AOB}	AOB decay rate	1/d	0.071-0.13	0.096		2,5,8, 9,19
NOB						
μ_{NOB}^{R2}	the maximum specific growth rate	1/d	0.38-1.44	1.44		2,3,5, 6,8,9, 16,17,19,
$K_{NO_2^-}^{R2}$	nitrite half saturation coefficient	g N/m^3	0.16-5.5	1.2		5,8,9, 16,19,22, 24
$K_{O_2}^{R2}$	oxygen half saturation coefficient	g O_2/m^3	0.16-2.2	0.74		2,5,6, 8,9,16, 19,22-25
b_{NOB}	NOB decay rate	1/d	0.06-0.096	0.096		2,5,8, 9,19
Heterotrophs						
μ_{H}^{R3}	heterotrophic maximum specific growth rate	1/d	2-6.25	6		1-3,8,9
K_{S}^{R3}	readily biodegradable substrate half saturation coefficient	g COD/m^3	2-20	2		1-3,5, 9,26,27
$K_{O_2,H}$	oxygen half saturation coefficient	g O_2/m^3	0.1-2	0.2		1-3,5, 8,9,26
b_H	aerobic heterotrophic	1/d	0.2-0.62	0.62		1-3,5, 9

Symbol	Definition	Unit	Reference range	Default	Calibrated	References
	decay rate					
HDB						
μ_{HDB}^{R4}	heterotrophic maximum specific growth rate	1/d	2-6.25	6		1-3,8,9
μ_{HDB}^{R5}	heterotrophic maximum specific growth rate	1/d	2-6.25	6		1-3,8,9
K_S^{R4}	readily biodegradable substrate half saturation coefficient	g COD/m^3	2-20	20		1-3,5, 9,26,27
K_S^{R5}	readily biodegradable substrate half saturation coefficient	g COD/m^3	2-20	2		1-3,5, 9,26,27
$K_{NO_3^-}^{R4}$	nitrate half saturation coefficient	g N/m^3	0.2-0.5	0.5		1-3,5, 8,9,26, 28
$K_{NO_2^-}^{R5}$	nitrite half saturation coefficient	g N/m^3	0.06-8	0.2		2,3,5, 8,9,26, 28
$K_{i,O_2,HDB}$	oxygen inhibition coefficient	g O_2/m^3	0.1-2	0.2		1-3,5, 8,9,26
η_g^{R4}	anoxic growth factor 1, reducing nitrate to nitrite	-	0.029-0.8	0.2		1-3,9,29
η_g^{R5}	anoxic growth factor 2, reducing nitrite to dinitrogen	-	0.075-0.81	0.6		2,3,9, 29,30
b_{HDB}	anoxic heterotrophic decay rate	1/d	0.2-0.62	0.62		1-3,5, 9
AnAOB						

Symbol	Definition	Unit	Reference range	Default	Calibrated	References
μ_{AnAOB}^{R6}	the maximum specific growth rate	1/d	0.019-0.14	0.03	0.14	3,16-17, 27,31-36
$K_{NH_4^+}^{R6}$	ammonia half saturation coefficient	g N/m^3	0.03-21	0.07		16,31,32, 34,37-39
$K_{NO_2^-}^{R6}$	nitrite half saturation coefficient	g N/m^3	0.005-2	0.05		16,31-34, 38,39,40
$K_{i,O,AnAOB}$	oxygen inhibition coefficient	g O_2/m^3	0.01-0.4	0.01	0.4	31,37,38
b_{AnAOB}	anammox bacteria decay rate	1/d	0.0003-0.016	0.003		3,27, 31-34
Hydrolysis						
k_h	maximum specific hydrolysis rate	1/d	1.5-4.5	3		1,2,5 9,30
K_X	slowly biodegradable substrate half saturation coefficient	g COD/g COD	0.03-1	0.03		1,2,5 9
η_{hANOX}	anoxic hydrolysis factor	-	0.4-0.8	0.4		1,2
Ammonification						
K_a	ammonification rate	m^3/g COD/d	0.08-0.1608	0.08		1,2

References: [1](Henze et al., 2000); [2](Hiatt and Grady, 2008); [3](Samie et al., 2011); [4](Law et al., 2012); [5](Ni et al., 2011); [6](Mampaey et al., 2013); [7](Hellinga et al., 1998); [8](Kampschreur et al., 2007); [9](Ni et al., 2013a); [10](Ni et al., 2013b); [11](Ni et al., 2014b); [12](Peng et al., 2015a and 2015b); [13](Pocquet et al., 2013); [14](Guo and Vanrolleghem, 2014); [15](Pocquet et al., 2016); [16](Van Hulle et al., 2012); [17](Ni et al., 2014a); [18](Mampaey et al., 2011); [19](Wiesmann et al., 1994); [20](Van Hulle et al., 2007); [21](Pynaert, 2003); [22](Cao et al., 2017); [23](Guisasola et al., 2005); [24](Hydromantis, 2014); [25](Isanta et al., 2015); [26](von Schulthess and Gujer, 1996); [27](Liu et al., 2016); [28](Pan et al., 2013); [29](Pan et al., 2015); [30](Mannina et al., 2018); [31](Koch et al., 2000); [32](Dapena-Mora et al., 2004); [33](Hao et al., 2002); [34](Ni et al., 2009); [35](Lotti et al., 2015); [36](Bae et al., 2010); [37](Strous et al., 1998); [38](Bi et al., 2015); [39](Stewart et al., 2017); [40](Lotti et al., 2014)

Table S6. Sensitivity coefficients calculated for the adjusted stoichiometric parameters.

	NH_4^+	NO_2^-	NO_3^-		NH_4^+	NO_2^-	NO_3^-
Y_{AOB}	**1.1240**	**-3.7559**	-0.0680	f_P	-0.0349	0.0053	0.0008
Y_{NOB}	-0.0024	**0.5836**	**-0.2832**	f_I	-0.0019	0.0552	0.0444
Y_H	0.0091	**-0.5809**	-0.0142	i_{XB}	**0.2848**	-0.0271	0.0001
Y_{HDB}	-0.0021	0.0040	0.0022	i_{XP}	0.0330	0.0044	-0.0011
Y_{AnAOB}	**0.5607**	**2.7116**	0.0459				

Table S7. Sensitivity coefficients calculated for the adjusted kinetic parameters.

	NH_4^+	NO_2^-	NO_3^-		NH_4^+	NO_2^-	NO_3^-
AOB							
μ_{AOB}^{R1}	**-1.2539**	**3.9972**	0.0734	$K_{O_2}^{R1}$	**0.3525**	**-1.2334**	-0.0066
$K_{NH_4^+}^{R1}$	0.0049	-0.0427	0.0009	b_{AOB}	0.0161	-0.0460	0.0003
NOB							
μ_{NOB}^{R2}	0.0016	**-0.6168**	**0.3008**	$K_{O_2}^{R2}$	-0.0009	**0.3368**	-0.1627
$K_{NO_2^-}^{R2}$	-0.0022	0.0505	-0.0224	b_{NOB}	0.0004	0.0073	-0.0049
Heterotrophs							
μ_{H}^{R3}	-0.0008	0.0005	0.0004	$K_{O_2,H}$	-0.0014	0.0119	0.0009
K_{S}^{R3}	0.0005	0.0010	0.0004	b_{H}	**0.2815**	0.1174	0.0003
HDB							
μ_{HDB}^{R4}	0.0000	0.0013	-0.0013	$K_{NO_2^-}^{R5}$	0.0000	0.0000	0.0000
μ_{HDB}^{R5}	0.0000	-0.0032	0.0000	$K_{i,O_2,HDB}$	-0.0014	0.0119	0.0009
K_{S}^{R4}	0.0005	0.0010	0.0004	η_{g}^{R4}	0.0000	0.0013	-0.0013
K_{S}^{R5}	0.0005	0.0010	0.0004	η_{g}^{R5}	0.0000	-0.0032	0.0000
$K_{NO_3^-}^{R4}$	0.0000	0.0000	0.0000	b_{HDB}	0.0004	0.0000	0.0000
AnAOB							
μ_{AnAOB}^{R6}	**-0.5824**	**-3.1105**	0.1033	$K_{i,O,AnAOB}$	-0.0870	**-0.4533**	0.0152
$K_{NH_4^+}^{R6}$	0.0024	0.0030	-0.0012	b_{AnAOB}	0.0007	0.0004	0.0000
$K_{NO_2^-}^{R6}$	0.0021	0.0122	-0.0014				
Hydrolysis							
k_{h}	-0.0057	-0.0272	-0.0015	η_{hANOX}	-0.0055	-0.0080	-0.0003
K_{X}	0.0033	0.0188	0.0009				
Ammonification							
K_{a}	**-0.8837**	-0.0038	0.0000				

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