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Title

A consilience model to describe N_2O production during biological N-removal

Author list

Carlos Domingo-Félez, Barth F. Smets*

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Supplementary Information

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4 Tables

Table S1 – Variability of selected parameters associated to biological N_2O models.

Parameter	Description	Units	Literature Range	References
η_{AOB}	Anoxic reduction factor	(-)	0.053 - 0.5	(1) (2) (3) (4)
K_{AOB_NO2}	NO_2^- affinity coefficient for denitrification	(mgN/L)	0.14 - 8	(5) (6) (7) (8)
K_{AOB_NO}	NO affinity coefficient for denitrification	(mgN/L)	0.004 - 0.1	(4) (5)
$K_{AOB\_i\_O2}$	O_2 inhibition coefficient for denitrification	(mgCOD/L)	0.078 - 0.112	(1) (2) (3) (4)
μ_{NIR}	Max. NO_2^- reduction rate	(h^{-1})	0.017 - 0.078	(3) (9) (10) (11)
μ_{NOR}	Max. NO reduction rate	(h^{-1})	0.038 - 0.345	(1) (3) (10) (11)
μ_{NOS}	Max. N_2O reduction rate	(h^{-1})	0.065 - 0.182	(3) (9) (10) (11)
$K_{HB\_i\_O2\_NIR}$	O_2 inhibition coefficient for NO_2^- denitrification	(mgCOD/L)	0.1 - 1	(9) (10) (11)
$K_{HB\_i\_O2\_NOR}$	O_2 inhibition coefficient for NO denitrification	(mgCOD/L)	0.067 - 1	(1) (3) (10) (11)
$K_{HB\_i\_O2\_NOS}$	O_2 inhibition coefficient for N_2O denitrification	(mgCOD/L)	0.031 - 1	(9) (10) (11)
$K_{HB\_S\_NIR}$	S_S affinity coefficient for NO_2^- denitrification	(mgCOD/L)	1.5 - 20	(9) (10) (11)
$K_{HB\_S\_NOR}$	S_S affinity coefficientfor NO denitrification	(mgCOD/L)	0.56 - 20	(1) (3) (10) (11)
$K_{HB\_S\_NOS}$	S_S affinity coefficient for N_2O denitrification	(mgCOD/L)	2 - 40	(9) (10) (11)

(1) - Ni et al. 2011, (2) - Ni et al. 2013a, (3) Ni et al. 2013b, (4) Spérandio et al. 2016, (5) Schreiber et al. 2009, (6) Kampschreur et al. 2007, (7) Mampaey et al. 2013, (8) Garnier et al. 2007, (9) von Schulthess et al. 1994, (10) Guo et al. 2013, (11) Hiatt and Grady 2008.

Table S2 – Stoichiometric matrix and process rates of relevant biological processes of the NDHA model.

Component (i) ▸ Process (j) ▾		1 S_S	2 S_{O2}	3 S_{NH3}	4 S_{NH2OH}	5 S_{HNO2}	6 S_{NO3}	7 S_{NO}	8 S_{N2O}	9 S_{N2}	10 $X_{B,AOB}$	11 $X_{B,NOB}$	12 $X_{B,H}$	13 X_S	14 X_I
AOB growth															
Aerobic_AMO	1		-1.14	-1	1										
Aerobic_HAO*	2			$-i_{NXB}$	$-\frac{1}{Y_{AOB}}$			$\frac{1}{Y_{AOB}}$			1				
Aerobic_HAO	3		$-\left(\frac{2.29-Y_{AOB}}{Y_{AOB}}\right)$	$-i_{NXB}$	$-\frac{1}{Y_{AOB}}$	$\frac{1}{Y_{AOB}}$					1				
Anox_A_NIR	4				-1	-3		4							
Anox_A_NOR	5				-1			-2	3						
NOB growth															
Aer_NOB_growth	6		$-\left(\frac{1.14-Y_{NOB}}{Y_{NOB}}\right)$	$-i_{NXB}$		$-\frac{1}{Y_{NOB}}$	$\frac{1}{Y_{NOB}}$					1			
HB growth															
Aerobic_H_growth	7	$-\frac{1}{Y_{HB}}$	$-\left(\frac{1-Y_{HB}}{Y_{HB}}\right)$	$-i_{NXB}$									1		
Anox_H_NAR	8	$-\frac{1}{Y_{HB}}$		$-i_{NXB}$		$\left(\frac{1-Y_{HB}}{1.14\cdot Y_{HB}}\right)$	$-\left(\frac{1-Y_{HB}}{1.14\cdot Y_{HB}}\right)$						1		
Anox_H_NIR	9	$-\frac{1}{Y_{HB}}$		$-i_{NXB}$		$-\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$		$\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$					1		
Anox_H_NOR	10	$-\frac{1}{Y_{HB}}$		$-i_{NXB}$				$-\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$	$\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$				1		
Anox_H_NOS	11	$-\frac{1}{Y_{HB}}$		$-i_{NXB}$					$-\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$	$\left(\frac{1-Y_{HB}}{0.57\cdot Y_{HB}}\right)$			1		
Lysis															
AOB	12			$i_{NXB}-f_I\cdot i_{NXI}-(1-f_I)\cdot i_{NXS}$							-1			$1-f_{XI}$	f_{XI}
NOB	13			$i_{NXB}-f_I\cdot i_{NXI}-(1-f_I)\cdot i_{NXS}$								-1		$1-f_{XI}$	f_{XI}
HB	14			$i_{NXB}-f_I\cdot i_{NXI}-(1-f_I)\cdot i_{NXS}$									-1	$1-f_{XI}$	f_{XI}
Hydrolysis															
Aerobic	15	1		i_{NXS}										-1	
Anoxic	16	1		i_{NXS}										-1	
Anaerobic	17	1		i_{NXS}										-1	
Abiotic N_2O_prod	18				x	y			z						

Component (i) ▸ / Process (j) ▼		Process Rate ($g \cdot m^{-3} \cdot s^{-1}$)
AOB growth		
Aerobic_AMO	*1*	$\mu_{AMO}^{AOB} \cdot \frac{S_{O2}}{S_{O2} + K_{O2\_AMO}^{AOB}} \cdot \frac{S_{NH3}}{S_{NH3} + K_{NH3}^{AOB}} \cdot \frac{S_{IC}}{S_{IC} + K_{IC}^{AOB}} \cdot X_{AOB}$
Aerobic_HAO*	*2*	$\mu_{HAO}^{AOB} \cdot \varepsilon \cdot \frac{S_{NH2OH}}{S_{NH2OH} + K_{NH2OH}^{AOB}} \cdot \frac{S_{IC}}{S_{IC} + K_{IC}^{AOB}} \cdot X_{AOB}$
Aerobic_HAO	*3*	$\mu_{HAO}^{AOB} \cdot (1-\varepsilon) \cdot \frac{S_{O2}}{S_{O2} + K_{O2\_HAO}^{AOB}} \cdot \frac{S_{NH2OH}}{S_{NH2OH} + K_{NH2OH}^{AOB}} \cdot \frac{S_{IC}}{S_{IC} + K_{IC}^{AOB}} \cdot X_{AOB}$
Anox_A_NIR	*4*	$\mu_{HAO}^{AOB} \cdot \eta_{NIR} \cdot \frac{K_{i\_O2}^{AOB}}{S_{O2} + K_{i\_O2}^{AOB}} \cdot \frac{S_{NH2OH}}{S_{NH2OH} + K_{NH2OH\_ND}^{AOB}} \cdot \frac{S_{HNO2}}{S_{HNO2} + K_{HNO2}^{AOB}} \cdot X_{AOB}$
Anox_A_NOR	*5*	$\mu_{HAO}^{AOB} \cdot \eta_{NOR} \cdot \frac{S_{NH2OH}}{S_{NH2OH} + K_{NH2OH}^{AOB}} \cdot \frac{S_{NO}}{S_{NO} + K_{NO}^{AOB}} \cdot X_{AOB}$
NOB growth		
Aer_NOB_growth	6	$\mu_{NOB} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}^{NOB}} \cdot \frac{S_{HNO2}}{S_{HNO2} + K_{O2}^{NOB}} \cdot \frac{S_{IC}}{S_{IC} + K_{IC}^{NOB}} \cdot X_{NOB}$
HB growth		
Aerobic_H_growth	7	$\mu_{HB} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}^{HB}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}^{HB}} \cdot \frac{S_S}{S_S + K_S^{HB}} \cdot X_{HB}$
Anox_H_NAR	8	$\mu_{NAR}^{HB} \cdot \frac{K_{i\_O2\_NAR}^{HB}}{S_{O2} + K_{i\_O2\_NAR}^{HB}} \cdot \frac{S_S}{S_S + K_{S\_NAR}^{HB}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}^{HB}} \cdot \frac{S_{NO3}}{S_{NO3} + K_{NO3}^{HB}} \cdot X_{HB}$
Anox_H_NIR	9	$\mu_{NIR}^{HB} \cdot \frac{K_{i\_O2\_NIR}^{HB}}{S_{O2} + K_{i\_O2\_NIR}^{HB}} \cdot \frac{K_{i\_NO\_NIR}^{HB}}{S_{NO} + K_{i\_NO\_NIR}^{HB}} \cdot \frac{S_S}{S_S + K_{S\_NIR}^{HB}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}^{HB}} \cdot \frac{S_{NO2}}{S_{NO2} + K_{NO2}^{HB}} \cdot X_{HB}$
Anox_H_NOR	10	$\mu_{NOR}^{HB} \cdot \frac{K_{i\_O2\_NOR}^{HB}}{S_{O2} + K_{i\_O2\_NOR}^{HB}} \cdot \frac{S_S}{S_S + K_{S\_NOR}^{HB}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}^{HB}} \cdot \frac{S_{NO}}{S_{NO} + K_{NO}^{HB} + S_{NO}{}^2 / K_{i\_NO\_NOR}^{HB}} \cdot X_{HB}$
Anox_H_NOS	11	$\mu_{NOS}^{HB} \cdot \frac{K_{i\_O2\_NOS}^{HB}}{S_{O2} + K_{i\_O2\_NOS}^{HB}} \cdot \frac{K_{i\_NO\_NOS}^{HB}}{S_{NO} + K_{i\_NO\_NOS}^{HB}} \cdot \frac{S_S}{S_S + K_{S\_NOS}^{HB}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}^{HB}} \cdot \frac{S_{N2O}}{S_{N2O} + K_{N2O}^{HB}} \cdot X_{HB}$
Lysis		
AOB	12	$b_{AOB} \cdot \left(\frac{S_{O2}}{S_{O2} + K_{O2\_b}^{AOB}} + \eta_b^{AOB} \cdot \frac{K_{O2\_b}^{AOB}}{K_{O2\_b}^{AOB} + S_{O2}} \cdot \frac{S_{NOx}}{K_{NOx}^{AOB} + S_{NOx}} \right) \cdot X_{AOB}$
NOB	13	$b_{NOB} \cdot (\ldots) \cdot X_{NOB}$
HB	14	$b_{HB} \cdot (\ldots) \cdot X_{HB}$
Hydrolysis		
Aerobic	15	$k_H \cdot \frac{X_S / X_{BH}}{K_X + X_S / X_{BH}} \cdot \frac{S_{O2}}{K_{O2}^{HB} + S_{O2}} \cdot X_{HB}$
Anoxic	16	$k_H \cdot \eta_{ANOX} \cdot \frac{X_S / X_{BH}}{K_X + X_S / X_{BH}} \cdot \frac{K_{O2}^{HB}}{K_{O2}^{HB} + S_{O2}} \cdot \frac{S_{NO3}}{K_{NO3}^{HB} + S_{NO3}} \cdot X_{HB}$
Anaerobic	17	$k_H \cdot \eta_{AN} \cdot \frac{X_S / X_{BH}}{K_X + X_S / X_{BH}} \cdot \frac{K_{O2}^{HB}}{K_{O2}^{HB} + S_{O2}} \cdot \frac{K_{NO3}^{HB}}{K_{NO3}^{HB} + S_{NO3}} \cdot X_{HB}$
Abiotic N_2O_prod	18	$k_{Abiotic\_1} \cdot S_{NH2OH} \cdot S_{HNO2};\ k_{Abiotic\_2} \cdot S_{NH2OH} \cdot f(pH)$

Table S3 – Reactions and processes of the NDHA model (AOB only).

Reaction	Location	
R1	AMO	$NH_3 + O_2 + 2H^+ + 2e^- \rightarrow NH_2OH + H_2O$
R2	HAO	$NH_2OH \rightarrow NO + 3H^+ + 3e^-$
R3	HAO	$NH_2OH + H_2O \rightarrow HNO_2 + 4H^+ + 4e^-$
R4	NIR	$3HNO_2 + 2H^+ + e^- \rightarrow NO + H_2O$
R5	NOR	$2NO + 2H^+ + 2e^- \rightarrow N_2O + H_2O$
R6	Cytaa3	$O_2 + 4H^+ \rightarrow 2H_2O$

Process	Reactions	
P1	R1	$NH_3 + O_2 + 2H^+ + 2e^- \rightarrow NH_2OH + H_2O$
P2	R2	$NH_2OH \rightarrow NO + 3H^+ + 3e^-$
P3	R3 + 0.5R6	$NH_2OH + 0.5O_2 \rightarrow HNO_2 + 2H^+ + 4e^-$
P4	R3 + 4R4	$NH_2OH + 3HNO_2 \rightarrow 4NO + 3H_2O$
P5	R2 + 1.5R5	$NH_2OH + 2NO \rightarrow 1.5N_2O + 1.5H_2O$

Table S4 – Parameters of two-pathway AOB models.

AOB_Model parameters	NN-ND Pocquet *et al.* 2016	NN-ND NDHA	NN-ND Ni *et al.* 2014	
μ_AMO	x	x	x	k_NH3_ox
μ_HAO	x	x	x	k_NH2OH_ox
η_NIR	x	x	x	k_NO_ox
η_NOR	x	x	x	k_O2_red
ε_AOB	-	x	x	k_NO2_red
K_O2_AMO	x	x	x	k_NO_red
K_O2_HAO	x	x	x	K_O2_NH3
K_O2_i	x	x	x	K_O2_red
K_O2_denit	x	-	x	K_NH3
K_NH3	x	x	x	K_NH2OH
K_NH2OH	x	x	x	K_NO_ox
K_NO	x	x	x	K_NO_red
K_NO_NN	x	-	x	K_NO2
K_HNO2	x	x	x	K_M_ox
K_NH2OH_ND	-	x	x	K_M_red,1
			x	K_M_red,2
			x	K_M_red,3
			x	K_M_red,4
Model_Parameters	13	13	18	

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