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Chapter 7
Supplementary Information

Table S1. The definition of all model components

Variable	Description
S_{O2}	Dissolved oxygen (DO) concentration
S_{NH3}	Ammonia (NH_3) concentration
S_{NH4}	Ammonium (NH_4^+) concentration
S_{NO2}	Nitrite (NO_2^-) concentration
S_{NO3}	Nitrate (NO_3^-) concentration
S_{N2}	Nitrogen gas (N_2) concentration
S_{HNO2}	Free nitrite acid (FNA) concentration
S_{NO}	Nitric oxide (NO) concentration
S_{N2O}	Nitrous oxide (N_2O) concentration
S_{NH2OH}	Hydroxylamine (NH_2OH) concentration
S_{NOH}	Nitrosyl radical (NOH) concentration
S_{Mred}	Reduced form of electron carrier (Mred) concentration
S_{Mox}	Oxidized form of electron carrier (Mox) concentration
S_{ADP}	Released form of energy carrier (ADP) concentration
S_{ATP}	Reserved form of energy carrier (ATP) concentration
S_{CO2}	Inorganic carbon (IC) concentration
S_S	Readily biodegradable COD concentration
X_H	Heterotrophic denitrifiers (HD) concentration
X_{AOB}	Ammonia-oxidizing bacteria (AOB) concentration

Table S2. Process matrices for the two types of four-step denitrification models describing N_2O production by heterotrophic denitrifiers

Process	Model components								Kinetic rate expressions
	S_{NO3}	S_{NO2}	S_{NO}	S_{N2O}	S_{N2}	S_S	S_{Mox}	S_{Mred} X_H	
Model OHO-A – ASMN, the "direct coupling approach" adapted from Hiatt and Grady (2008)									
1	$-\frac{1-Y_H\cdot\eta_Y}{1.143\cdot Y_H\cdot\eta_Y}$	$\frac{1-Y_H\cdot\eta_Y}{1.143\cdot Y_H\cdot\eta_Y}$				$-1/(Y_H\cdot\eta_Y)$		1	$\mu_H\eta_{g1}(\frac{S_S}{K_{S1}+S_S})(\frac{S_{NO3}}{K^{HB}_{NO3}+S_{NO3}})X_H$
2		$-\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$	$\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$			$-1/(Y_H\cdot\eta_Y)$		1	$\mu_H\eta_{g2}(\frac{S_S}{K_{S2}+S_S})(\frac{S_{NO2}}{K^{HB}_{NO2}+S_{NO2}})(\frac{K_{NO,2}}{K_{NO,2}+S_{NO}})X_H$
3			$-\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$	$\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$		$-1/(Y_H\cdot\eta_Y)$		1	$\mu_H\eta_{g3}(\frac{S_S}{K_{S3}+S_S})(\frac{S_{NO}}{K^{HB}_{NO}+S_{NO}+S^2_{NO}/K_{NO,3}})X_H$
4				$-\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$	$\frac{1-Y_H\cdot\eta_Y}{0.571\cdot Y_H\cdot\eta_Y}$	$-1/(Y_H\cdot\eta_Y)$		1	$\mu_H\eta_{g4}(\frac{S_S}{K_{S4}+S_S})(\frac{S_{N2O}}{K^{HB}_{N2O}+S_{N2O}})(\frac{K_{NO,4}}{K_{NO,4}+S_{NO}})X_H$
Model OHO-B – ASM-ICE, the "indirect coupling approach" adapted from Pan *et al.* (2013b)									
1						-1	$-(1-Y_H)$	$1-Y_H$ Y_H	$r_{COD,\max}(\frac{S_S}{K_S+S_S})(\frac{S_{Mox}}{K_{Mox}+S_{Mox}})X_H$
2	-1	1					1	-1	$r_{NO3,\max}(\frac{S_{NO3}}{K^{HB}_{NO3}+S_{NO3}})(\frac{S_{Mred}}{K_{Mred,1}+S_{Mred}})X_H$
3		-1	1				$\frac{1}{2}$	$-\frac{1}{2}$	$r_{NO2,\max}(\frac{S_{NO2}}{K^{HB}_{NO2}+S_{NO2}})(\frac{S_{Mred}}{K_{Mred,2}+S_{Mred}})X_H$
4			-1	$\frac{1}{2}$			$\frac{1}{2}$	$-\frac{1}{2}$	$r_{NO,\max}(\frac{S_{NO}}{K^{HB}_{NO}+S_{NO}})(\frac{S_{Mred}}{K_{Mred,3}+S_{Mred}})X_H$
5				-1	1		1	-1	$r_{N2O,\max}(\frac{S_{N2O}}{K^{HB}_{N2O}+S_{N2O}})(\frac{S_{Mred}}{K_{Mred,4}+S_{Mred}})X_H$
									$S_{Mred}+S_{Mox}=C_{tot}$

Table S3. Process matrices for the six single-pathway N_2O models of AOB in literature

Process	Model components								Kinetic rate expressions
	S_{O2}	S_{NH4} (S_{NH3})	S_{NH2OH}	S_{NOH}	S_{NO2} (S_{HNO2})	S_{NO}	S_{N2O}	X_{AOB}	
Model A – AOB denitrification pathway (Ni *et al.*, 2011)									
A-1	-1.14	-1	1						$\mu_{AOB,AMO}\frac{S_{O2}}{K_{O2,AOB,1}+S_{O2}}\frac{S_{NH4}}{K_{NH4,AOB}+S_{NH4}}X_{AOB}$
A-2	$-\frac{2.29-Y_{AOB}}{Y_{AOB}}$	$-i_{N,AOB}$	$-\frac{1}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$			1	$\mu_{AOB,HAO}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
A-3			-1		-3	4			$\eta_{AOB}\mu_{AOB,HAO}\frac{K_{I,O2,AOB}}{S_{O2}+K_{I,O2,AOB}}\frac{S_{NO2}}{K_{NO2,AOB}+S_{NO2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
A-4			-1		1	-4	4		$\eta_{AOB}\mu_{AOB,HAO}\frac{K_{I,O2,AOB}}{S_{O2}+K_{I,O2,AOB}}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
Model A1 – AOB denitrification pathway (Pocquet *et al.*, 2013)									
A1-1	-1.14	-1	1						$\mu_{AOB,AMO}\frac{S_{O2}}{K_{O2,AOB,1}+S_{O2}}\frac{S_{NH3}}{K_{NH3,AOB}+S_{NH3}+(S_{NH3})^2/K_{I,NH3,AOB}}X_{AOB}$
A1-2	$-\frac{2.29-Y_{AOB}}{Y_{AOB}}$	$-i_{N,AOB}$	$-\frac{1}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$			1	$\mu_{AOB,HAO}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
A1-3			-1		-3	4			$\eta_{AOB}\mu_{AOB,HAO}\frac{S_{HNO2}}{K_{HNO2,AOB}+S_{HNO2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
A1-4			-1		1	-4	4		$\eta_{AOB}\mu_{AOB,HAO}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
Model B – AOB denitrification pathway (Mampaey *et al.*, 2013)									
B-1	$-\frac{3.43-Y_{AOB}}{Y_{AOB}}$	$-\frac{1}{Y_{AOB}}-i_{N,AOB}$			$\frac{1}{Y_{AOB}}$			1	$\mu_{AOB}\frac{S_{O2}}{K_{O2,AOB}+S_{O2}}\frac{S_{NH3}}{K_{NH3,AOB}+S_{NH3}}X_{AOB}$
B-2	$-\frac{2.29-Y_{AOB,den}}{Y_{AOB,den}}$	$-\frac{1}{Y_{AOB,den}}-i_{N,AOB}$			$-\frac{1}{Y_{AOB,den}}$	$\frac{2}{Y_{AOB,den}}$		1	$\eta_{AOB}\mu_{AOB}\frac{S_{O2}}{K_{O2,AOB}+S_{O2}}\frac{S_{NH3}}{K_{NH3,AOB}+S_{NH3}}\frac{S_{HNO2}}{K_{HNO2,AOB}+S_{HNO2}}X_{AOB}$

(***Continued***)

B-3	$-\frac{2.29-Y_{AOB,den}}{Y_{AOB,den}}$	$-\frac{1}{Y_{AOB,den}}-i_{N,AOB}$		$\frac{1}{Y_{AOB,den}}$	$-\frac{2}{Y_{AOB,den}}$	$\frac{2}{Y_{AOB,den}}$	1	$\eta_{AOB}\mu_{AOB}\frac{S_{O2}}{K_{O2,AOB}+S_{O2}}\frac{S_{NH3}}{K_{NH3,AOB}+S_{NH3}}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}X_{AOB}$
Model B1 – AOB denitrification pathway (Guo and Vanrolleghem, 2014)								
B1-1	$-\frac{3.43-Y_{AOB}}{Y_{AOB}}$	$-\frac{1}{Y_{AOB}}-i_{N,AOB}$		$\frac{1}{Y_{AOB}}$			1	$\mu_{AOB}\frac{S_{O2}}{K_{O2,AOB}+S_{O2}}\frac{S_{NH3}}{K_{NH3,AOB}+S_{NH3}+(S_{NH3})^2/K_{I,NH3,AOB}}\frac{K_{I,HNO2,AOB}}{K_{I,HNO2,AOB}+S_{HNO2}}X_{AOB}$
B1-2	$-\frac{2.29-Y_{AOB,den}}{Y_{AOB,den}}$	$-\frac{1}{Y_{AOB,den}}-i_{N,AOB}$		$-\frac{1}{Y_{AOB,den}}$	$\frac{2}{Y_{AOB,den}}$		1	$\eta_{AOB}\mu_{AOB}\frac{S_{NH3}}{K_{NH3,AOB,den}+S_{NH3}}\frac{S_{HNO2}}{K_{HNO2,AOB}+S_{HNO2}}X_{AOB}DO_{Haldane}$
B1-3	$-\frac{2.29-Y_{AOB,den}}{Y_{AOB,den}}$	$-\frac{1}{Y_{AOB,den}}-i_{N,AOB}$		$\frac{1}{Y_{AOB,den}}$	$-\frac{2}{Y_{AOB,den}}$	$\frac{2}{Y_{AOB,den}}$	1	$\eta_{AOB}\mu_{AOB}\frac{S_{NH3}}{K_{NH3,AOB,den}+S_{NH3}}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}X_{AOB}DO_{Haldane}$
								$DO_{Haldane}=\frac{S_{O2}}{K_{O2,AOB,den}+(1-2\sqrt{K_{O2,AOB,den}/K_{I,O2,AOB}})S_{O2}+(S_{O2})^2/K_{I,O2,AOB}}$
Model C – NH_2OH/NOH pathway (Law *et al.*, 2012)								
C-1	-1.14	-1	1					$\mu_{AOB,AMO}\frac{S_{O2}}{K_{O2,AOB,1}+S_{O2}}\frac{S_{NH4}}{K_{NH4,AOB}+S_{NH4}}X_{AOB}$
C-2	$-\frac{1.14-Y_{AOB}}{Y_{AOB}}$	$-i_{N,AOB}$	$-\frac{1}{Y_{AOB}}$	$\frac{1}{Y_{AOB}}$			1	$\mu_{AOB,HAO,1}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
C-3	– 1.14			-1	1			$\mu_{AOB,HAO,2}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NOH}}{K_{NOH,AOB}+S_{NOH}}X_{AOB}$
C-4				-1			1	$k_{NOH}S_{NOH}$
Model D – NH_2OH/NO pathway (Ni *et al.*, 2013b)								
D-1	-1.14	-1	1					$\mu_{AOB,AMO}\frac{S_{O2}}{K_{O2,AOB,1}+S_{O2}}\frac{S_{NH4}}{K_{NH4,AOB}+S_{NH4}}X_{AOB}$
D-2	$-\frac{1.71-Y_{AOB}}{Y_{AOB}}$	$-i_{N,AOB}$	$-\frac{1}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$		1	$\mu_{AOB,HAO,1}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$
D-3	– 0.57			1	-1			$\mu_{AOB,HAO,2}\frac{S_{O2}}{K_{O2,AOB,2}+S_{O2}}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}X_{AOB}$
D-4			-1	1	-4	4		$\eta_{AOB}\mu_{AOB,HAO,1}\frac{S_{NO}}{K_{NO,AOB}+S_{NO}}\frac{S_{NH2OH}}{K_{NH2OH,AOB}+S_{NH2OH}}X_{AOB}$

Table S4. Process matrices for the two-pathway N_2O models of AOB in literature

Process	Model components												Kinetic rate expressions
	S_{O2}	S_{NH4} (S_{NH3})	S_{NH2OH}	S_{NO2}	S_{NO}	S_{N2O}	S_{Mox}	S_{Mred}	S_{ADP}	S_{ATP}	S_{CO2}	X_{AOB}	
Model E – Decoupling approach, electron balance based model (Ni *et al.*, 2014)													
E-1	-1	-1	1				1	-1					$r_{NH4,ox}\frac{S_{O2}}{K_{O2,NH4}+S_{O2}}\frac{S_{NH4}}{K_{NH4}+S_{NH4}}\frac{S_{Mred}}{K_{Mred,1}+S_{Mred}}X_{AOB}$
E-2			-1		1		-3/2	3/2					$r_{NH2OH,ox}\frac{S_{NH2OH}}{K_{NH2OH}+S_{NH2OH}}\frac{S_{Mox}}{K_{Mox}+S_{Mox}}X_{AOB}$
E-3				1	-1		-1/2	1/2					$r_{NO,ox}\frac{S_{NO}}{K_{NO,ox}+S_{NO}}\frac{S_{Mox}}{K_{Mox}+S_{Mox}}X_{AOB}$
E-4					-1	1/2	1/2	-1/2					$r_{NO,red}\frac{S_{NO}}{K_{NO,red}+S_{NO}}\frac{S_{Mred}}{K_{Mred,2}+S_{Mred}}X_{AOB}$
E-5	-1/2						1	-1					$r_{O2,red}\frac{S_{O2}}{K_{O2,red}+S_{O2}}\frac{S_{Mred}}{K_{Mred,3}+S_{Mred}}X_{AOB}$
E-6				-1		1/2	1	-1					$r_{NO2,red}\frac{S_{NO2}}{K_{NO2}+S_{NO2}}\frac{S_{Mred}}{K_{Mred,4}+S_{Mred}}X_{AOB}$
													$S_{Mred}+S_{Mox}=C_{tot}$
Model F – Decoupling approach, electron and ATP balance based model (Peng *et al.*, 2015a)													
F-1	-1	-1	1				1	-1	-2/3	2/3			$r_{NH4,ox}\frac{S_{O2}}{K_{O2,NH4}+S_{O2}}\frac{S_{NH4}}{K_{NH4}+S_{NH4}}\frac{S_{Mred}}{K_{Mred,1}+S_{Mred}}\frac{S_{ADP}}{K_{ADP}+S_{ADP}}X_{AOB}$
F-2			-1		1		-1	1					$r_{NH2OH,ox}\frac{S_{NH2OH}}{K_{NH2OH}+S_{NH2OH}}\frac{S_{Mox}}{K_{Mox}+S_{Mox}}X_{AOB}$
F-3				1	-1		-1	1					$r_{NO,ox}\frac{S_{NO}}{K_{NO,ox}+S_{NO}}\frac{S_{Mox}}{K_{Mox}+S_{Mox}}X_{AOB}$
F-4					-1	1/2							$r_{NO,red}S_{NO}$

F-5	-1/2					1	-1	-1/3	1/3		$r_{O2,red}\frac{S_{O2}}{K_{O2,red}+S_{O2}}\frac{S_{Mred}}{K_{Mred,2}+S_{Mred}}\frac{S_{ADP}}{K_{ADP}+S_{ADP}}X_{AOB}$
F-6			-1		1/2	1	-1	-1/3	1/3		$r_{NO2,red}\frac{S_{NO2}}{K_{NO2}+S_{NO2}}\frac{S_{Mred}}{K_{Mred,3}+S_{Mred}}\frac{S_{ADP}}{K_{ADP}+S_{ADP}}X_{AOB}$
F-7						2	-2	15	-15	-1	1	$r_{AOB}\frac{S_{CO2}}{K_{CO2}+S_{CO2}}\frac{S_{Mred}}{K_{Mred,4}+S_{Mred}}\frac{S_{ATP}}{K_{ATP}+S_{ATP}}X_{AOB}$
											$S_{Mred}+S_{Mox}=C_{tot,1}$
											$S_{ADP}+S_{ATP}=C_{tot,2}$
Model G – Coupling approach, model G (Pocquet *et al.*, 2016)											
G-1	-8/7	-1	1								$q_{AOB,AMO}\frac{S_{O_2}}{S_{O_2}+K_{O_2,AOB,1}}\frac{S_{NH_3}}{S_{NH_3}+K_{NH_3,AOB}}X_{AOB}$
G-2	$-\frac{12/7-Y_{AOB}}{Y_{AOB}}$	$-i_{N,BM}$	$-\frac{1}{Y_{AOB}}$		$\frac{1}{Y_{AOB}}$					1	$\mu_{AOB,HAO}\frac{S_{O_2}}{S_{O_2}+K_{O_2,AOB,2}}\frac{S_{NH_2OH}}{S_{NH_2OH}+K_{NH_2OH,AOB}}\frac{S_{NH4}}{S_{NH4}+10^{-12}}X_{AOB}$
G-3	-4/7			1	-1						$q_{AOB,HAO}\frac{S_{O_2}}{S_{O_2}+K_{O_2,AOB,2}}\frac{S_{NO}}{S_{NO}+K_{NO,AOB,HAO}}X_{AOB}$
G-4			-1	1	-4	4					$q_{AOB,N2O,NN}\frac{S_{NH_2OH}}{S_{NH_2OH}+K_{NH_2OH,AOB}}\frac{S_{NO}}{S_{NO}+K_{NO,AOB,NN}}X_{AOB}$
G-5			-1	-1		2					$q_{AOB,N2O,ND}\frac{S_{NH_2OH}}{S_{NH_2OH}+K_{NH_2OH,AOB}}\frac{S_{HNO_2}}{S_{HNO_2}+K_{HNO_2,AOB}}f(S_{O2})X_{AOB}$
											$f(S_{O2})=\frac{S_{O_2}}{K_{O_2,AOB,ND}+(1-2\cdot\sqrt{K_{O_2,AOB,ND}/K_{I,O_2,AOB}})\cdot S_{O_2}+S_{O_2}^2/K_{I,o_2,AOB}}$
											$q_{AOB,AMO}=q_{AOB,HAO}=\mu_{AOB}/Y_{AOB}$
											$q_{AOB,N2O,NN}=\eta_{AOB,NN}.q_{AOB,HAO}$
											$q_{AOB,N2O,ND}=\eta_{AOB,ND}.q_{AOB,HAO}$