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Modeling nitrous oxide emissions from agricultural soil incubation experiments using CoupModel

Jie Zhang et al.

Correspondence to: Jie Zhang (jiezh@agro.au.dk)

Table S1: Summary of calibration data sets. Values in the brackets show the standard deviation of each time series measurements.

No	Treatment	Mean values of discrete measurements					Cumulative gas fluxes and mean mineral N derived from integration over sampling period				
		N_2O	CO_2	NH_4^+	NO_3^-	NO	N_2O	CO_2	NH_4^+	NO_3^-	NO
	Units	g N m^{-2} day^{-1}	g C m^{-2} day^{-1}	g N m^{-2}	g N m^{-2}	g N m^{-2} day^{-1}	g N m^{-2}	g C m^{-2}	g N m^{-2}	g N m^{-2}	g N m^{-2}
	Mix RC										
1	40 % WFPS, -NO_3^-	0.002 (0.003)	3.46 (4.01)	0.37 (0.55)	-	-	0.059	88.6	0.34	-	-
2	40 % WFPS, +NO_3^-	0.003 (0.003)	3.12 (3.51)	0.40 (0.45)	-	-	0.067	80.7	0.34	-	-
3	60 % WFPS, -NO_3^-	0.021 (0.044)	4.08 (3.43)	0.53 (0.32)	-	-	0.340	126	0.60	-	-
4	60 % WFPS, +NO_3^-	0.161 (0.442)	4.10 (3.78)	0.58 (0.33)	-	9×10^{-4} (0.003)	3.968	129	0.53	-	0.012
	Control RC										
5	40 % WFPS, -NO_3^-	1×10^{-4} (4×10^{-5})	0.32 (0.30)	0.018 (0.016)	1.14 (0.17)	-	0.005	14.3	0.011	1.19	-
6	40 % WFPS, +NO_3^-	4×10^{-4} (0.001)	0.21 (0.17)	0.013 (0.006)	6.21 (0.39)	-	0.014	7.41	0.011	6.11	-
7	60 % WFPS, -NO_3^-	0.005 (0.012)	0.99 (0.87)	0.018 (0.010)	1.11 (0.11)	-	0.118	36.1	0.015	1.13	-
8	60 % WFPS, +NO_3^-	0.004 (0.009)	0.73 (0.80)	0.012 (0.006)	5.78 (0.21)	2×10^{-4} (6×10^{-5})	0.100	23.5	0.011	5.84	0.007
	Mix WW										
9	40 % WFPS, -NO_3^-	4×10^{-5} (3×10^{-5})	1.53 (0.66)	0.012 (0.010)	-	-	0.002	55.5	0.008	-	-
10	40 % WFPS, +NO_3^-	8×10^{-4} (4×10^{-4})	1.87 (0.88)	0.029 (0.030)	-	-	0.031	71.2	0.018	-	-
11	60 % WFPS, -NO_3^-	7×10^{-4} (0.001)	1.89 (0.63)	0.019 (0.027)	-	-	0.015	71.1	0.008	-	-
12	60 % WFPS, +NO_3^-	0.001 (0.001)	2.10 (0.87)	0.020 (0.016)	-	1×10^{-4} (3×10^{-4})	0.029	79.8	0.014	-	0.002
	Control WW										

13	40 % WFPS, $-NO_3^-$	3×10^{-5} (1×10^{-5})	0.19 (0.06)	0.005 (0.004)	1.09 (0.20)	-	0.001	7.26	0.004	1.16	-
14	40 % WFPS, $+NO_3^-$	2×10^{-4} (8×10^{-5})	0.12 (0.08)	0.014 (0.012)	6.48 (0.46)	-	0.007	4.25	0.011	6.27	-
15	60 % WFPS, $-NO_3^-$	9×10^{-5} (5×10^{-5})	0.19 (0.06)	0.006 (0.006)	1.09 (0.12)	-	0.004	7.42	0.004	1.11	-
16	60 % WFPS, $+NO_3^-$	1×10^{-4} (7×10^{-5})	0.13 (0.08)	0.006 (0.006)	5.83 (0.22)	2×10^{-4} (6×10^{-5})	0.005	5.10	0.004	5.84	0.007
Measurement occasions (n)		10[a]	10[a]	4[b]	4[b]	10[a]					

[a]Samples were taken at day 1, 3, 6, 9, 13, 16, 22, 29, 36 and 43 of incubation.

[b]Samples were taken at day 1, 6, 22, and 43 of incubation.

Table S2: Parameters and equations related to the study. Equation indices refer to the manual (Jansson and Karlberg, 2010) and the bracketed "updated" equations are described based on the update log in the manual and model interface.

No	Parameter name	Process	Unit	Equation	Description	Related process in Fig. 1
1	k_{l1}	SOM decompositon	day^{-1}	(6.3) $C_{DecompL} = k_l\, f(T)\, f(\theta)\, C_{litter}$ where $C_{DecompL}$ is the decomposition rate of litter pool. $f(T)$ and $f(\theta)$ is the common response function for soil temperature and soil moisture. C_{litter} is the size of litter pool (litter 1 or litter 2). Changing k_l to k_h and C_{litter} to C_{humus} gives the decomposition rate of humus pool.	Rate coefficient for the decay of C in litter 1 (the active SOC pool and the plant metabolic C pool).	c1-c3, n1-n3
2	k_{l2}	SOM decompositon	day^{-1}	(6.3)	Rate coefficient for the decay of C in litter 2 (the slow SOC pool and the plant structural C pool).	c6-c8, n4-n6
3	k_h	SOM decompositon	day^{-1}	(6.3)	Rate coefficient for the decay of C in humus (the passive SOC pool).	c10, n7
4	cn_m	SOM decompositon	-	(6.7) $N_{Litter\rightarrow Humus} = C_{Litter\rightarrow Humus}/cn_m$ (6.8) $N_{Litter\rightarrow NH_4} = C_{DecompL}\left(\frac{1}{CN_{Litter}} - \frac{f_{e,l}}{cn_m}\right)$ Soil mineralization/immobilization of N, where CN_{Litter} is the C/N ratio in litter pool. Changing $C_{DecompL}$ to $C_{DecompH}$, $f_{e,l}$ to $f_{e,h}$ and CN_{Litter} to CN_{Humus} gives the flow from the humus pool. A negative value means net immobilization.	A fixed C-N ratio of microbes used in the calculations of mineralization and immobilization.	n1-n7, n11

5	$f_{e,l1}$	SOM decompositon	-	(6.4) $C_{Litter\rightarrow CO_2} = (1 - f_{e,l}) \cdot C_{DecompL}$ (6.8)	Efficiency parameter of the decay of the active SOM pool and the plant metabolic material pool. (1- $f_{e,l1}$) is the fraction of decomposed C mineralized to CO_2.	c1-c3, n1-n3
6	$f_{e,l2}$	SOM decompositon	-	(6.4) (6.8)	Efficiency of the decay of the slow SOM pool and the plant structural material pool. (1- $f_{e,l2}$) is the fraction of decomposed C mineralized to CO_2.	c6-c8, n4-n6
7	$f_{e,h}$	SOM decompositon	-	(6.4) (6.8)	Efficiency of the decay of the passive SOM pool. (1- $f_{e,h}$) is the fraction of decomposed C mineralized to CO_2.	c10, n7
8	$f_{h,l1}$	SOM decompositon	-	(6.5) $C_{Litter\rightarrow Humus} = f_{e,l} f_{h,l} C_{DecompL}$ (6.6) $C_{Litter\rightarrow Litter} = f_{e,l}(1 - f_{h,l}) \cdot C_{DecompL}$ The C fluxes from litter pool decomposition to humus pool and to litter pool respectively.	Fraction of the C and N contained in the active SOM pool and the plant metabolic material pool that will enter the passive pool.	c2-c3, n1-n2
9	$f_{h,l2}$	SOM decompositon	-	(6.5) (6.6)	Fraction of the C and N contained in the slow SOM pool and the plant structural material pool that will enter the passive pool.	c6-c7, n5-n6
10	θ_{wilt}	Soil hydrology	vol %	(5.86) $f(\theta) = \begin{cases} p_{\theta satact} & \theta = \theta_s \\ min\left(\left(\frac{\theta_s - \theta}{p_{\theta Upp}}\right)^{p_{\theta p}} (1 - p_{\theta satact}) + p_{\theta satact}, \left(\frac{\theta - \theta_{wilt}}{p_{\theta Low}}\right)^{p_{\theta p}}\right) & \theta_{wilt} < \theta < \theta_s \\ 0 & \theta < \theta_{wilt} \end{cases}$	Wilting point in soil moisture response function.	c1-c10, n1-n11, n22-24

11	$i_{nitrmicr}$	Nitrification	gN m^{-2}	(6.26) $N_{micrN} = i_{nitmicr} \cdot n_{dist}$ where N_{micrN} is the initial biomass of nitrifiers in each layer and n_{dist} is a distribution function for the profile in the form of a linear function or an exponential function or a constant.	The initial biomass of nitrifiers for the whole soil profile.	Initial nitrifier biomass in each layer
12	$n_{hrateNH4}$	Nitrification	mg N L^{-1}	(6.57) $f\left(N_{NH_4\ Cons}\right) = \frac{N_{NH_4}/(\theta \cdot \Delta z)}{(N_{NH_4}/(\theta \cdot \Delta z))+n_{hrateNH4}}$ The response function for soil ammonium concentration for nitrification.	The parameter describing the ammonium concentration for half rate in the response function for ammonium concentration.	n8
13	$n_{micrate}$	Nitrification	mg ha/(day kg)	(6.56) $N_{NH_4 \to NO_3} = n_{micrate}\, f(T) f(\theta) f\left(N_{NH_4\ Cons}\right) n_{pH} N_{micrN}$ where $N_{NH_4 \to NO_3}$ is the nitrification flux, N_{micrN} is the biomass of nitrifiers, $f\left(N_{NH_4\ Cons}\right)$ is the response function for soil ammonium concentration, n_{pH} is a parameter accounting for soil pH.	The nitrification rate coefficient in nitrification function when microbes are accounted for.	n8
14	$d_{denitrdie}$	Denitrification	day^{-1}	(6.50)	The death rate coefficient of denitrifiers.	n21
15	$d_{growthN2O}$	Denitrification	day^{-1}	(6.41) $N_{N_2O \to micrDN} = d_{growthN_2O} \cdot f\left(N_{NO_3Concinhib}\right) \cdot f\left(C_{DO,dnCons}\right) \cdot f\left(N_{NxOyConc}\right) \cdot M_{activity} \cdot N_{micrDN}$ The losses of N_2O from the anaerobic nitrogen pool due to microbial growth, where $M_{activity}$ is the microbial activity of denitrifiers, $f\left(N_{NO_3Concinhib}\right)$ is an inhibition response function for the nitrate content, and $f\left(C_{DO,dnCons}\right)$ and $f\left(N_{NxOyConc}\right)$ are response functions for dissolved organics and nitrogen concentration respectively.	The growth parameter in the denitrification function describing the loss of N_2O from the anaerobic nitrogen pool due to microbial growth.	n19
16	$d_{growthNO}$	Denitrification	day^{-1}	(6.41) $N_{NO \to micrDN} = d_{growthNO} \cdot f\left(C_{DO,dnCons}\right) \cdot f\left(N_{NxOyConc}\right) \cdot M_{activity} \cdot N_{micrDN}$ The losses of NO from the anaerobic nitrogen pool due to microbial growth. Changing $d_{growthNO}$ to $d_{growthNO2}$ or $d_{growthNO3}$ gives the losses of NO_2^- or NO_3^- respectively.	The growth parameter in the denitrification function describing the loss of NO from the anaerobic nitrogen pool due to microbial growth.	n17
17	$d_{growthNO2}$	Denitrification	day^{-1}	(6.41)	The growth parameter in the denitrification function describing the loss of NO_2^- from the anaerobic nitrogen pool due to microbial growth.	n15
18	$d_{growthNO3}$	Denitrification	day^{-1}	(6.41)	The growth parameter in the denitrification	n13

					function describing the loss of NO_3^- from the anaerobic nitrogen pool due to microbial growth.	
19	$d_{actratecoef}$	Denitrification	day^{-1}	(6.51) $M_{activity} = f(T) \cdot f(pH) \cdot f(N_{AnTot}) \cdot f_{Anvol}(z) \cdot d_{actratecoef}$ The activity of denitrifiers, where $f(T)$, $f(pH)$ and $f(N_{AnTot})$ are response functions for soil temperature, pH and total nitrogen content in the anaerobic nitrogen pools respectively and $f_{Anvol}(z)$ is the anaerobic fraction.	The denitrification activity rate coefficient in denitrifer activity function.	Denitrifier activity
20	$d_{pHhrate}$	Denitrification	-	(6.51) (6.52) $f(pH) = 1 - \frac{1}{1+e^{(pH-d_{pHhrate})/d_{pHhhape}}}$ The response function for soil pH in the denitrification process, where $d_{pHhhape}$ is a shape parameter.	The pH half rate in denitrifier activity function	Denitrifier activity
28	$i_{denitmicr}$	Denitrification	$gN\ m^{-2}$	(6.26) $N_{micrDN} = i_{denitmicr} \cdot d_{dist}$ where N_{micrDN} is the initial biomass of denitrifiers in each layer and d_{dist} is a distribution coefficient that varies with depth.	The initial biomass of denitrifiers for the whole soil profile.	Initial denitrifier biomass in each layer
21	$d_{inhihrate}$	Denitrification	$mg\ N\ L^{-1}$	(6.42) $f(N_{NO_3\ \mathrm{Concinhib}}) = \frac{d_{\mathrm{inhihrate}}}{d_{\mathrm{inhihrate}} + N_{NO_3\ \mathrm{Conc}}}$ The inhibition response function for nitrate content in the soil that effect the growth of denitrifiers during N_2O formation.	The denitrification inhibition half rate of NO_3^- that effect the growth of denitrification microbes during N_2O formation.	n19
22	$d_{hrateNxOy}$	Denitrification	$mg\ N\ L^{-1}$	(6.44) $f(N_{NxOyConc}) = \frac{N_{NxOyconc}}{d_{hrateNxOy} + N_{NxOyConc}}$ The response function for nitrogen concentratiaon for denitrification.	The parameter describing the nitrogen concentration for half rate in the NxOy denitrification process	n13, n15, n17, n19, n20
23	d_{effN2O}	Denitrification	-	(6.47) $N_{rgN_2O} = N_{AnN_2O \to micrDN}/d_{effN_2O} - N_{AnN_2O \to micrDN}$ The growth respiration of denitrifers for N_2O, where $N_{AnN_2O \to micrDN}$ is the losses of N_2O from the anaerobic nitrogen pool due to microbial growth (eq. 1.30). Changing $N_{AnN_2O \to micrDN}$ to $N_{AnNO \to micrDN}$, $N_{AnNO2 \to micrDN}$ or $N_{AnNO3 \to micrDN}$, and changing d_{effN_2O} to d_{effNO}, d_{effNO2} or d_{effNO3} gives the respiration based on NO, NO_2^- or NO_3^- respectively.	The efficiency parameter in the growth respiration function for N_2O.	n18
24	d_{effNO}	Denitrification	-	(6.47)	The efficiency parameter in the growth	n16

					respiration function for NO.	
25	d_{effNO2}	Denitrification	-	(6.47)	The efficiency parameter in the growth respiration function for NO_2^-.	n14
26	d_{effNO3}	Denitrification	-	(6.47)	The efficiency parameter in the growth respiration function for NO_3^-.	n12
27	$d_{rc}N_2O$	Denitrification	day^{-1}	(6.48) $N_{rmN_2O} = \frac{d_{rcN_2O} \cdot N_{N_2O}}{N_{AnTot}}$ The maintenance respiration of denitrifiers for N_2O, where N_{AnTot} is the total nitrogen content in the N_2O, NO, NO_2^- and NO_3^- pools, and N_{N_2O} is the nitrogen content in the N_2O pool. Changing d_{rcN_2O} to d_{rcNO}, d_{rcNO2} or d_{rcNO3}, and changing N_{N_2O} to N_{NO}, N_{NO2} or N_{NO3} gives the respiration based on NO, NO_2^- or NO_3^- respectively.	The respiration coefficient in the denitrification function describing the maintenance respiration for N_2O.	n18
28	d_{rcNO}	Denitrification	day^{-1}	(6.48)	The respiration coefficient in the denitrification function describing the maintenance respiration for NO.	n16
29	d_{rcNO2}	Denitrification	day^{-1}	(6.48)	The respiration coefficient in the denitrification function describing the maintenance respiration for NO_2^-.	n14
30	d_{rcNO3}	Denitrification	day^{-1}	(6.48)	The respiration coefficient in the denitrification function describing the maintenance respiration for NO_3^-.	n12
31	$d_{denitrdiedormancy}$	Denitrification	day^{-1}	(6.50) (updated) $M_{death,DN} = d_{denitrdie} \cdot \max(N_{micrDN} - d_{denitrdiedormthres}, 0) + d_{denitrdiedormancy} \cdot N_{micrDN}$ The death rate of denitrifiers, where N_{micrDN} is the biomass of denitrifiers.	The death rate coefficient of denitrifiers during the entire range of microbial biomass	n21
32	$d_{denitrdiedormthres}$	Denitrification	g N^{-1} m^{-2}	(6.50)	The threshold of the amount of denitrifiers from which the death rate of denitrifiers will	n21

					be determined by the previous rate coefficient $d_{denitrdie}$.	
33	$g_{aporshape}$	Gas processes	-	(6.99) $f_{Anvol} = e^{-g_{aporshape} \cdot O_{volcons}^2}$ where f_{Anvol} is the volumetric anaerobic fraction of soil, $g_{aporshape}$ is a shape parameter and $O_{volcons}$ is the volumetric oxygen concentration.	The shape parameter as a function of oxygen level in the volumetric anaerobic fraction of the soil.	g3
34	d_{O2}	Gas processes	-	(6.72) $O_{diffrate} = d_{O_2} \cdot f_a \cdot o_{O_2\ diffrate} \cdot D_O$ where $O_{diffrate}$ is the oxygen diffusion rate, $o_{O_2\ diffrate}$ is the oxygen diffusion rate at 20 °C, D_O is the diffusion coefficient in free air and f_a is the air porosity.	The tortuosity parameter in the calculation of oxygen diffusion rate.	O_2 diffusion rate
35	$d_{actpower}$	Gas processes	-	(6.51) (updated) $d(f_{Anvol}) = f_{Anvol}^{d_{actpower}}$ The response function for denitrifers to anaerobic fraction.	Power coefficient of denitrifiers response to anaerobic fraction	g4
36	$o_{diffred}$	Gas processes	-	(6.71) $f(O_2) = o_{diffred} \cdot f_{Anvol} \cdot (1 - f_{Anvol}) \cdot O_{diffrate} + o_b$ The oxygen diffusion exchange function used to calculate the diffusion of N trace gases from anaerobic fraction to aerobic fraction.	The oxygen diffusion reduction parameter in the oxygen diffusion exchange function.	g5
37	o_b	Gas processes	-	(6.71)	Base level of oxygen diffusion function	g5
38	$g_{mfracNO}$	Gas processes	-	(6.64) $N_{NO_3 \to NO} = g_{mfracNO} \cdot f(\theta) \cdot f(T) \cdot f(pH) \cdot N_{NH_4 \to NO_3}$ The NO flux from the nitrification process, where $N_{NH_4 \to NO_3}$ is the nitrification rate, $f(\theta)$, $f(T)$ and $f(pH)$ are the response functions for soil moisture, temperature and pH respectively. Changing $g_{mfracNO}$ to $g_{mfracN2O}$ gives the N_2O flux from the nitrification process.	The maximum NO fraction parameter when NO is formed during the nitrification process	n25
39	$g_{\theta satcritNO}$	Gas processes	-	(6.65) $f(\theta)_{NO} = 1 - \frac{1}{1+e^{(\theta(z)/\theta_S(z) - g_{\theta satritNO})/g_{\theta satormNO}}}$ The response function for soil moisture for NO formation during the nitrification process, where $\theta(z)$ is the soil moisture content, $\theta_s(z)$ is the water content at saturation, and $g_{\theta satritNO}$ and $g_{\theta satormNO}$ are parameters. Changing $g_{\theta satritNO}$ to $g_{\theta satritN2O}$, and $g_{\theta satormNO}$ to $g_{\theta satormN2O}$ gives the response function for soil moisture for N_2O formation during the nitrification process.	The relative saturation level in the response function for soil moisture when NO is formed during the nitrification process.	n25
40	$g_{\theta satformNO}$	Gas processes		(6.65)	The parameter describing the shape of the moisture response function for NO during the nitrification process.	n25
41	$g_{mfrac}N_2O$	Gas processes	-	(6.64)	The maximum N_2O fraction parameter when N_2O is formed	n26

					during the nitrification process	
42	$g_{\theta satcrit}N_2O$	Gas processes	-	(6.65)	The relative saturation level in the response function for soil moisture when N_2O is formed during the nitrification process.	n26
43	$g_{\theta satform}N_2O$	Gas processes	-	(6.65)	The parameter describing the shape of the moisture response function for N_2O during the nitrification process.	n26
44	$p_{\theta Low}$	Common abiotic responses	vol %	(5.86)	Water content interval in the soil moisture response function for microbial activity, mineralisation-immobilisation, nitrification and denitrification.	c1-c10, n1-n11, n22-24
45	t_{Q10}	Common abiotic responses	-	(5.82) $f(T) = t_{Q10}^{(T-t_{Q10bas})/10}$	Response to a 10 °C soil temperature change on the microbial activity, mineralisation-immobilisation, nitrification and denitrification.	c1-c10, n1-n24

Table S3: Model performances of 20,000 simulations (prior) and around 50 accepted simulations (posteriors). Units: CO_2 flux (g C m^{-2} day^{-1}), N_2O flux (g N m^{-2} day^{-1}), NO flux (g N m^{-2} day^{-1}), NH_4^+ (g N m^{-2}), NO_3^- (g N m^{-2}), valid for the statistics of ME.

Treatment	Number of accepted runs	Calibrated variables	Prior						Posterior						Selection criteria		
			ME			R^2			ME			R^2			ME		R^2
			Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Min	Max	Min
1	42	CO_2	1.56	-3.42	16.0	0.85	0.61	0.99	-1.59	-3.31	2.29	0.70	0.62	0.98	-3.42	3.42	

		N_2O	-2.4E-03	-2.4E-03	0.03	0.59	3.5E-07	0.93	-1.6E-03	-2.3E-03	0.01	0.35	1.2E-03	0.80	-2.4E-03	0.01	
		NO															
		NH_4^+	5.31	-0.36	20.1	0.15	1.6E-09	1.00	0.05	-0.36	0.79	0.28	2.3E-03	1.00	-0.36	0.80	
		NO_3^-															
2	63	CO_2	1.90	-3.08	16.3	0.84	0.59	1.00	-0.15	-1.18	1.92	0.74	0.61	0.98	-1.20	2.00	
		N_2O	-1.8E-03	-2.6E-03	0.15	0.41	8.7E-08	0.95	-1.4E-04	-2.4E-03	4.9E-03	0.45	0.20	0.82	-2.4E-03	0.01	0.20
		NO															
		NH_4^+	5.09	-0.40	20.0	0.34	1.8E-06	1.00	-0.01	-0.38	0.48	0.66	0.01	1.00	-0.39	0.50	
		NO_3^-															
3	58	CO_2	1.54	-4.02	15.4	0.81	0.57	0.87	-1.95	-3.85	2.48	0.77	0.70	0.86	-4.00	4.00	
		N_2O	-0.01	-0.01	0.02	0.57	1.4E-06	1.00	-0.01	-0.01	-4.7E-03	0.23	0.01	0.75	-0.01	0.01	
		NO															
		NH_4^+	5.71	-0.53	20.0	0.08	1.2E-07	0.99	0.01	-0.33	0.28	0.32	6.5E-04	0.75	-0.33	0.28	
		NO_3^-															
4	37	CO_2	1.53	-4.04	16.2	0.61	0.31	0.67	2.21	0.19	4.92	0.56	0.33	0.67	-4.04	5.00	
		N_2O	-0.15	-0.16	-0.01	0.10	2.7E-07	1.00	-0.14	-0.16	-0.02	0.52	0.40	0.97	-0.16	0.16	0.40
		NO	0.01	-9.3E-04	0.21	0.13	4.9E-07	1.00	3.0E-03	-8.8E-04	0.01	0.28	2.5E-06	1.00	-8.8E-04	0.01	
		NH_4^+	3.08	-0.58	19.6	0.47	0.0E+00	1.00	0.10	-0.42	1.43	0.51	0.12	1.00	-0.42	1.50	
		NO_3^-															
5	40	CO_2	0.88	-0.32	11.8	0.02	2.0E-10	0.05	-0.01	-0.18	0.43	0.03	6.0E-04	0.05	-0.18	0.48	
		N_2O	-3.6E-05	-6.7E-05	0.03	0.06	7.6E-09	0.36	1.8E-04	-6.5E-05	1.6E-03	0.12	0.05	0.27	-6.5E-05	1.9E-03	
		NO															
		NH_4^+	1.44	-0.01	14.0	0.36	4.8E-07	1.00	0.02	-0.01	0.06	0.31	2.1E-04	0.91	-0.01	0.06	
		NO_3^-	-0.18	-0.94	0.20	0.96	1.0E-05	1.00	-0.29	-0.91	-0.18	0.90	0.17	1.00	-0.92	0.20	
6	67	CO_2	0.99	-0.21	11.9	0.02	2.0E-10	0.05	-0.05	-0.19	0.20	0.03	6.0E-04	0.05	-0.20	0.20	
		N_2O	-4.4E-05	-3.5E-04	0.12	0.06	7.6E-09	0.36	-5.7E-05	-3.0E-04	5.0E-04	0.12	0.05	0.27	-3.0E-04	6.0E-04	
		NO															
		NH_4^+	1.36	-0.01	14.0	0.36	4.8E-07	1.00	4.7E-03	-0.01	0.02	0.31	2.1E-04	0.91	-0.01	0.02	
		NO_3^-	0.46	-4.02	0.88	0.96	1.0E-05	1.00	0.33	-0.57	0.50	0.90	0.17	1.00	-0.60	0.60	
7	52	CO_2	0.59	-0.98	11.4	0.28	0.03	0.38	-0.41	-0.72	0.84	0.32	0.09	0.38	-0.72	0.84	
		N_2O	-4.5E-03	-4.5E-03	0.03	0.16	1.9E-08	0.99	-4.0E-03	-4.5E-03	4.0E-03	0.17	0.01	0.41	-4.5E-03	4.5E-03	

		NO															
		NH_4^+	1.85	-0.02	14.3	0.03	0.0E+00	1.00	0.02	-0.02	0.05	0.20	3.4E-04	0.98	-0.02	0.05	
		NO_3^-	-0.08	-0.88	0.36	0.93	0.0E+00	1.00	-0.13	-0.39	0.14	0.88	0.04	0.99	-0.40	0.36	
8	47	CO_2	0.85	-0.72	11.7	0.36	0.08	0.42	0.08	-0.22	0.89	0.37	0.13	0.42	-0.22	0.90	
		N_2O	-3.4E-03	-3.6E-03	0.14	0.13	8.2E-10	0.88	-2.0E-03	-3.6E-03	0.01	0.23	0.10	0.42	-3.6E-03	0.01	0.10
		NO	1.2E-04	-1.8E-04	0.12	0.61	8.4E-09	0.98	-4.6E-05	-1.8E-04	5.5E-04	0.68	0.01	0.97	-2.0E-04	6.0E-04	
		NH_4^+	1.79	-0.01	14.3	0.40	2.9E-07	1.00	0.03	-0.01	0.08	0.31	0.02	0.99	-0.01	0.08	
		NO_3^-	-0.31	-4.41	0.15	0.79	5.3E-04	1.00	-0.48	-2.25	-0.22	0.81	0.29	0.98	-2.50	0.15	
9	59	CO_2	1.84	-1.53	17.2	0.71	0.31	0.81	-0.07	-0.76	0.98	0.80	0.73	0.81	-0.79	1.00	
		N_2O	-1.1E-05	-3.6E-05	0.02	0.47	6.1E-09	0.78	-2.6E-05	-3.5E-05	4.8E-05	0.43	2.9E-04	0.63	-3.5E-05	5.0E-05	
		NO															
		NH_4^+	1.39	-0.01	14.4	0.85	4.5E-05	1.00	-2.0E-03	-0.01	0.01	0.76	2.6E-03	1.00	-0.01	0.01	
		NO_3^-															
10	46	CO_2	1.50	-1.87	16.8	0.46	0.07	0.69	0.03	-0.87	1.48	0.54	0.25	0.68	-0.87	1.50	
		N_2O	-4.4E-04	-7.8E-04	0.13	0.22	1.4E-08	0.69	2.5E-05	-4.3E-04	8.0E-04	0.16	2.7E-04	0.46	-4.3E-04	8.0E-04	
		NO															
		NH_4^+	1.33	-0.03	14.4	0.49	3.1E-07	1.00	-7.4E-04	-0.01	0.03	0.29	4.3E-04	0.97	-0.01	0.03	
		NO_3^-															
11	41	CO_2	2.56	-1.84	16.9	0.62	0.25	0.79	0.34	-1.15	1.58	0.72	0.49	0.79	-1.15	1.60	
		N_2O	-5.0E-04	-5.3E-04	0.03	0.56	2.1E-08	0.99	-4.8E-05	-5.1E-04	0.01	0.35	0.11	0.85	-5.1E-04	0.01	0.10
		NO															
		NH_4^+	1.92	-0.02	14.7	0.61	3.6E-07	1.00	-4.3E-03	-0.01	0.02	0.55	3.6E-07	1.00	-0.02	0.02	
		NO_3^-															
12	54	CO_2	2.35	-2.05	16.7	0.32	0.06	0.61	0.04	-1.82	1.92	0.44	0.17	0.60	-2.00	2.00	
		N_2O	-7.0E-04	-9.8E-04	0.15	0.40	3.1E-08	0.99	-3.3E-04	-8.9E-04	1.2E-03	0.27	0.10	0.76	-9.0E-04	1.5E-03	0.10
		NO	2.9E-04	-8.9E-05	0.13	0.29	2.2E-09	0.99	1.3E-03	-8.8E-05	0.02	0.33	0.03	0.94	-8.9E-05	0.02	
		NH_4^+	1.86	-0.02	14.7	0.85	2.2E-07	1.00	1.0E-03	-0.01	0.01	0.34	9.5E-06	0.99	-0.01	0.01	
		NO_3^-															
13	39	CO_2	1.01	-0.19	11.9	0.43	0.14	0.52	-0.02	-0.12	0.22	0.51	0.39	0.52	-0.12	0.25	
		N_2O	4.6E-06	-2.0E-05	0.03	0.33	1.2E-08	0.80	2.1E-05	-1.9E-05	2.3E-04	0.37	1.3E-03	0.67	-1.9E-05	2.5E-04	
		NO															

		NH_4^+	1.42	-2.7E-03	14.0	0.79	5.9E-05	1.00	0.01	-2.3E-03	0.02	0.59	0.02	1.00	-2.3E-03	0.02
		NO_3^-	-0.24	-0.90	0.14	0.73	0.0E+00	1.00	-0.27	-0.84	-0.24	0.75	1.9E-03	0.94	-0.90	0.14
14	49	CO_2	1.09	-0.11	12.0	0.26	8.2E-04	0.45	-0.02	-0.11	0.11	0.42	0.33	0.45	-0.11	0.12
		N_2O	1.5E-04	-1.8E-04	0.13	0.44	6.3E-08	0.84	4.6E-05	-6.6E-05	2.0E-04	0.23	1.4E-04	0.65	-7.0E-05	2.0E-04
		NO														
		NH_4^+	1.37	-0.01	14.0	0.63	2.3E-07	0.99	1.2E-03	-0.01	0.02	0.46	0.01	0.85	-0.01	0.02
		NO_3^-	0.57	-4.23	0.99	0.37	1.3E-07	1.00	0.46	-0.54	0.61	0.48	0.13	0.82	-0.99	0.99
15	39	CO_2	1.40	-0.17	12.2	0.18	3.5E-03	0.34	0.08	-0.16	0.48	0.28	0.02	0.34	-0.17	0.50
		N_2O	-3.6E-05	-6.3E-05	0.03	0.61	4.2E-09	0.91	-3.9E-06	-6.0E-05	2.5E-04	0.41	1.3E-03	0.84	-6.0E-05	3.0E-04
		NO														
		NH_4^+	1.85	-2.1E-03	14.3	0.56	8.3E-05	1.00	0.02	-2.1E-03	0.05	0.36	8.3E-05	1.00	-2.1E-03	0.05
		NO_3^-	-0.08	-0.86	0.35	0.97	0.0E+00	1.00	-0.14	-0.43	-0.08	0.92	0.03	0.99	-0.50	0.35
16	49	CO_2	1.45	-0.12	12.3	0.22	0.13	0.24	0.03	-0.10	0.20	0.24	0.22	0.24	-0.12	0.20
		N_2O	1.2E-04	-1.3E-04	0.15	0.12	0.0E+00	0.45	1.2E-05	-1.2E-04	5.6E-04	0.14	1.8E-07	0.40	-1.2E-04	6.0E-04
		NO	1.4E-04	-1.8E-04	0.12	0.60	6.6E-07	0.98	2.2E-04	-1.8E-04	1.9E-03	0.65	0.02	0.91	-1.8E-04	2.0E-03
		NH_4^+	1.80	-3.2E-03	14.3	0.55	1.5E-09	1.00	1.6E-03	-3.2E-03	0.01	0.68	2.8E-03	1.00	-3.2E-03	0.01
		NO_3^-	-0.21	-4.44	0.25	0.87	4.2E-06	1.00	-0.27	-0.83	-0.17	0.82	0.27	0.98	-1.00	1.00

Table S4: Model inputs and parameters used in the sensitivity analysis. Parameters intervals were defined as the default range in the model unless otherwise specified.

Parameter	Unit	Description	Range	
			min	max
Input parameters				
n_{soil}	%	Bulk soil porosity (measured: 52.8 %)	40	60
$n_{residue}$	%	Crop residue porosity (estimated: 86 %)	50	90
SOC_{l1}	-	Fraction of labile carbon pool in soil (estimated: 0.02)	0.001	0.1
SOC_h	-	Fraction of recalcitrant carbon pool in soil (estimated: 0.44)	0.3	0.64
ROC_{l1}	-	Fraction of labile organic carbon pool in residue (estimated: 0.82 for red clover and 0.55 for winter wheat)	0.3	0.85
pH	-	Soil pH value (measured: 6.18)	5.5	6.5
Process parameters				
Common abiotic responses				
$t_{Q10}{}^{a*}$	-	Response to a 10 °C soil temperature change on the microbial activity.	1.5	3
$p_{\theta Low}{}^{*}$	vol %	Lower value coefficient in the soil moisture response function	3	20
Soil hydrology				
$\theta_{wilt}{}^{b*}$	vol %	Wilting point in soil moisture response function	5	20
Gas processes				
$g_{aporshape}$	-	Shape parameter in the volumetric anaerobic fraction of the soil	1	500
$d_{O2}{}^{*}$	-	Tortuosity parameter in the calculation of oxygen diffusion rate	0.3	1
$d_{actpower}$	-	Power coefficient of denitrifiers response to anaerobic fraction	1	5
$o_{diffred}{}^{*}$	-	Reduction parameter in the oxygen diffusion exchange function	1E-04	1
$o_b{}^{*}$	-	Base level of oxygen diffusion function	1E-05	1
$g_{mfracN2O}$	-	Maximum N_2O fraction during the nitrification process	1E-04	0.1
$g_{mfracNO}$	-	Maximum NO fraction parameter during the nitrification process	1E-04	0.5
$g_{\theta satcritN2O}$	-	Relative saturation level in soil moisture response function for N_2O formation by nitrification	0.1	1
$g_{\theta satformN2O}$	-	Shape parameter in moisture response function for N_2O formation by nitrification	0.001	1
$g_{\theta satcritNO}$	-	Relative saturation level in soil moisture response function for NO formation by nitrification	0.1	1
$g_{\theta satformNO}$	-	Shape parameter in soil moisture response function for NO by nitrification	0.001	1

Denitrification				
$d_{inhibrate}^{*}$	mg N L^{-1}	Denitrification inhibition half rate of NO_3^- during N_2O formation	0.1	100
$d_{pHhrate}^{a*}$	-	pH half rate in denitrifier activity function	4	6
$d_{hrateNxOy}^{*}$	mg N L^{-1}	Nitrogen concentration half rate in the N_xO_y denitrification process	1	500
$d_{actratecoef}$	day^{-1}	Rate coefficient of denitrifier activity	0.1	1
$d_{denitrdiedormancy}$	day^{-1}	Death rate coefficient of denitrifiers during the entire range of microbial biomass	1E-06	0.01
$d_{denitrdie}$	day^{-1}	Death rate coefficient of denitrifiers.	1E-05	1
$d_{denitrdiedormthres}$	g N^{-1} m^{-2}	Threshold parameter in the denitrfier death function.	1E-05	0.1
d_{effN2O}^{*}	-	Efficiency parameter in the growth respiration function for N_2O	0.1	1
d_{effNO}^{*}	-	Efficiency parameter in the growth respiration function for NO	0.1	1
d_{effNO2}^{*}	-	Efficiency parameter in the growth respiration function for NO_2^-	0.1	1
d_{effNO3}^{*}	-	Efficiency parameter in the growth respiration function for NO_3^-	0.1	1
$d_{growthN2O}^{*}$	day^{-1}	Growth parameter describing the loss of N_2O from the anaerobic nitrogen pool	0.1	100
$d_{growthNO}^{*}$	day^{-1}	Growth parameter describing the loss of NO from the anaerobic nitrogen pool	0.1	100
$d_{growthNO2}^{*}$	day^{-1}	Growth parameter describing the loss of NO_2^- from the anaerobic nitrogen pool	0.1	100
$d_{growthNO3}^{*}$	day^{-1}	Growth parameter describing the loss of NO_3^- from the anaerobic nitrogen pool	0.1	100
d_{rcN2O}	day^{-1}	Maintenance respiration coefficient for N_2O	0.1	100
d_{rcNO}	day^{-1}	Maintenance respiration coefficient for NO	0.1	100
d_{rcNO2}	day^{-1}	Maintenance respiration coefficient for NO_2^-	0.1	100
d_{rcNO3}	day^{-1}	Maintenance respiration coefficient for NO_3^-	0.1	100
$i_{denitmicr}^{c*}$	g N m^{-2}	Initial biomass of denitrifiers for the whole soil profile	0.01	1
Nitrification				
$i_{nitrmicr}^{c*}$	g N m^{-2}	Initial biomass of nitrifiers for the whole soil profile	0.01	1
$n_{micrate}^{*}$	mg ha day^{-1} kg^{-1}	Nitrification rate coefficient in nitrification function	1E-06	1
$n_{hrateNH4}^{*}$	mg N L^{-1}	Ammonium half rate in the response function for ammonium concentration.	0.1	50
Soil organic processes				
cn_m^{d*}	-	Microbial C/N ratio used in the calculation of mineralization and immobilization	5	35
$f_{e,h}$	-	Efficiency of the decay of humus	0.1	0.8

$f_{e,l1}^{*}$	-	Efficiency of the decay of the litter 1 pool	0.1	0.8
$f_{e,l2}^{*}$	-	Efficiency of the decay of the litter 2 pool	0.1	0.8
$f_{h,l1}$	-	Fraction of the C converting from litter 1 to humus	0.1	0.9
$f_{h,l2}$	-	Fraction of the C converting from litter 2 to humus	0.1	0.9
k_h^{e}	day^{-1}	Rate coefficient for the decay of C in humus	1E-07	1E-04
k_{l1}^{e*}	day^{-1}	Rate coefficient for the decay of C in litter 1	0.001	0.5
k_{l2}^{e*}	day^{-1}	Rate coefficient for the decay of C in litter 2	1E-05	0.1

Superscript a: Intervals estimated from (Saleh-Lakha et al., 2009).

Superscript b: Intervals estimated from (Rai et al., 2017).

Superscript c: A safety factor of 0.1-20 was used to define the interval based on the default values in the model (scaled by the soil thickness).

Superscript d: Intervals estimated from (Nylinder et al., 2011).

Superscript e: Intervals estimated from (Gijsman et al., 2002).

[*] Parameters used in calibration.

Table S5: Initial sizes of organic C and N pools for the bulk soil, red clover and winter wheat. The bulk density of soil is 1250 kg m^{-3}, and the height of soil matrix is 0.04 m. The application rate of residues is 0.4 kg m^{-2}.

	C (g m^{-2})				N (g m^{-2})				C/N			
	Total	Litter1	Litter2	Humus	Total	Litter1	Litter2	Humus	Total	Litter1	Litter2	Humus
Soil	752[a]	15.0[b]	406[b]	331[b]	74.5[a]	1.1	26.1	47.3	10.1[a]	14[b]	15.6	7[b]
RC	179[a]	147[b]	32.2[b]	0[b]	10[a]	9.84	0.16	0	17.9[a]	14.9	200[b]	7[b]
WW	182[a]	100[b]	81.8[b]	0[b]	2[a]	1.59	0.41	0	90.9[a]	62.8	200[b]	7[b]

[a]Measured values; [b]Assumed values. Other values were calculated from measured values and assumed values. The initial partitioning ratio of organic carbon were assumed: for bulk soil, L1:L2:H = 0.02:0.54:0.44; for red clover (RC), L1:L2 = 0.82:0.18; for winter wheat (WW), L1:L2 = 0.55:0.45. The predefined C/N ratios refers to (Gijsman et al., 2002).

Table S6: Comparison of modeled cumulative N_2O fluxes between single-layer model and multiple-layer model (STD: standard deviation). Unit: g N m^{-2}.

Treatment	Measured	Simulated: single-layer model[a]		Simulated: multiple-layer model	
	Mean	Mean	STD	Mean	STD

mix RC					
40 % WFPS, -NO3	0.059	0.041	0.080	0.021	0.074
40 % WFPS, +NO3	0.067	0.132	0.128	0.109	0.108
60 % WFPS, -NO3	0.340	0.012	0.043	0.002	0.020
60 % WFPS, +NO3	3.968	0.716	0.863	0.747	0.720
control RC					
40 % WFPS, -NO3	0.005	0.010	0.018	0.005	0.013
40 % WFPS, +NO3	0.014	0.015	0.012	0.015	0.010
60 % WFPS, -NO3	0.118	0.024	0.066	3×10^{-5}	2×10^{-4}
60 % WFPS, +NO3	0.100	0.072	0.123	0.014	0.047
mix WW					
40 % WFPS, -NO3	0.002	4×10^{-4}	0.001	3×10^{-4}	0.001
40 % WFPS, +NO3	0.031	0.041	0.017	0.040	0.019
60 % WFPS, -NO3	0.015	0.026	0.074	0.005	0.009
60 % WFPS, +NO3	0.029	0.034	0.031	0.021	0.025
control WW					
40 % WFPS, -NO3	0.001	0.002	0.003	0.001	0.002
40 % WFPS, +NO3	0.007	0.011	0.005	0.010	0.004
60 % WFPS, -NO3	0.004	0.003	0.004	9×10^{-5}	2×10^{-4}
60 % WFPS, +NO3	0.005	0.007	0.008	0.010	0.009

[a]Single-layer model calibrated by individual treatment

55 [b]Single-layer model calibrated by multiple treatments

Table S7: The mean of simulated oxygen, anaerobic fraction, N_2O sources and biomass for 16 treatments in the posterior models.

No	Volumetric oxygen content[a] (%)	Volumetric anaerobic fraction[a] (%)	Percentrage of cumulative N_2O (denitrificaiton) (%)	Percentrage of cumulative N_2O (nitrificaiton) (%)
1	19.92	1.89	99.98	0.02
2	19.86	1.93	99.99	0.01
3	19.85	1.94	76.34	23.66

4	19.52	2.28	100	0.002
9	19.99	1.84	99.88	0.12
10	19.99	1.83	100	0.002
11	19.96	1.86	85.49	14.51
12	19.94	1.87	96.61	3.39
13	19.94	1.87	98.99	1.01
14	19.92	1.89	100	0.004
15	19.88	1.92	99.99	0.01
16	19.87	1.93	99.99	0.01
21	19.99	1.84	99.76	0.24
22	20.00	1.83	100	0.001
23	19.98	1.84	99.95	0.05
24	19.99	1.84	99.99	0.01
Average	19.91	1.90	97.31	2.69

[a] The average volumetric oxygen content and the average volumetric anaerobic fraction over the ten sampling days.

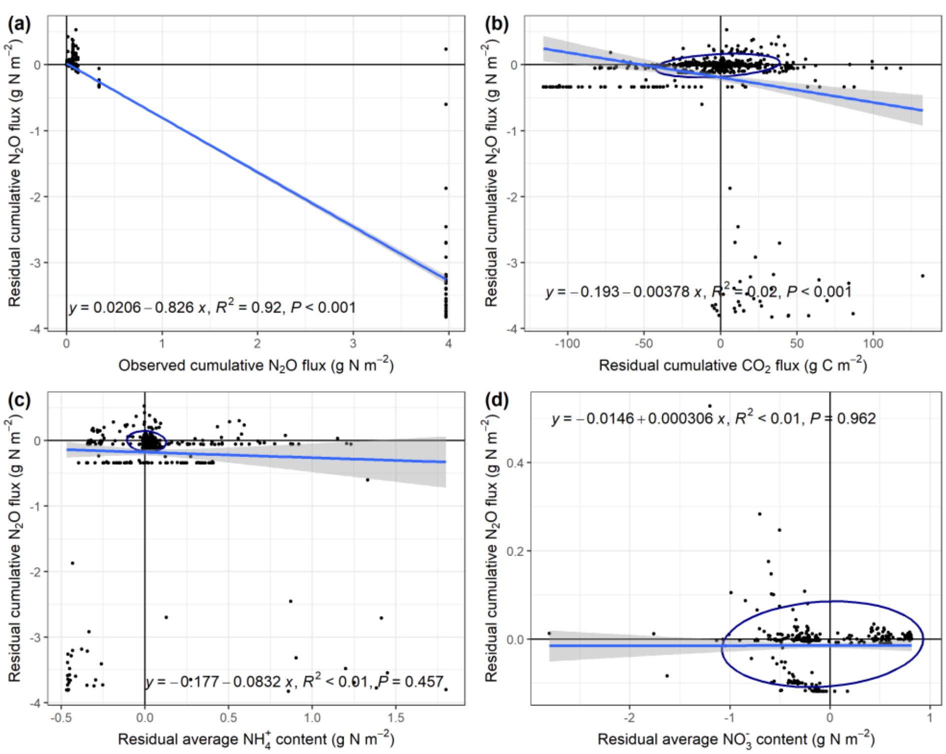


Figure S1: Scatter plots with linear regressions and 95 % uncertainty bands for the residuals of cumulative N_2O flux against (a) the observed cumulative N_2O fluxes, (b) the cumulative CO_2 residuals, (c) the average soil NH_4^+ residuals, and (d) the average soil NO_3^- residuals, respectively.

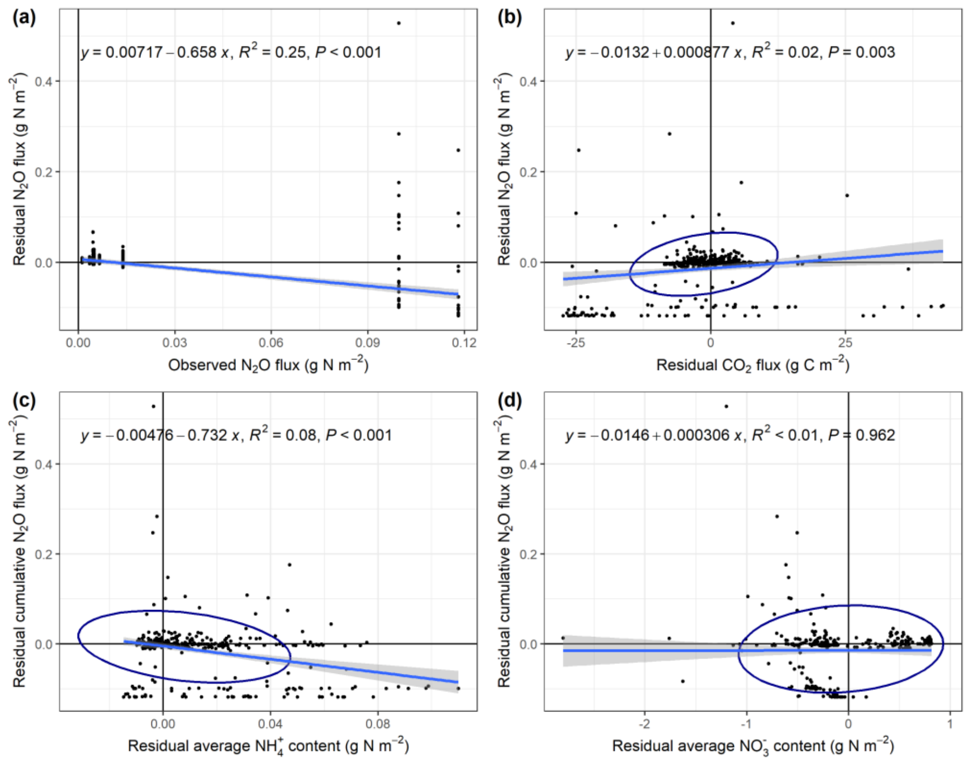
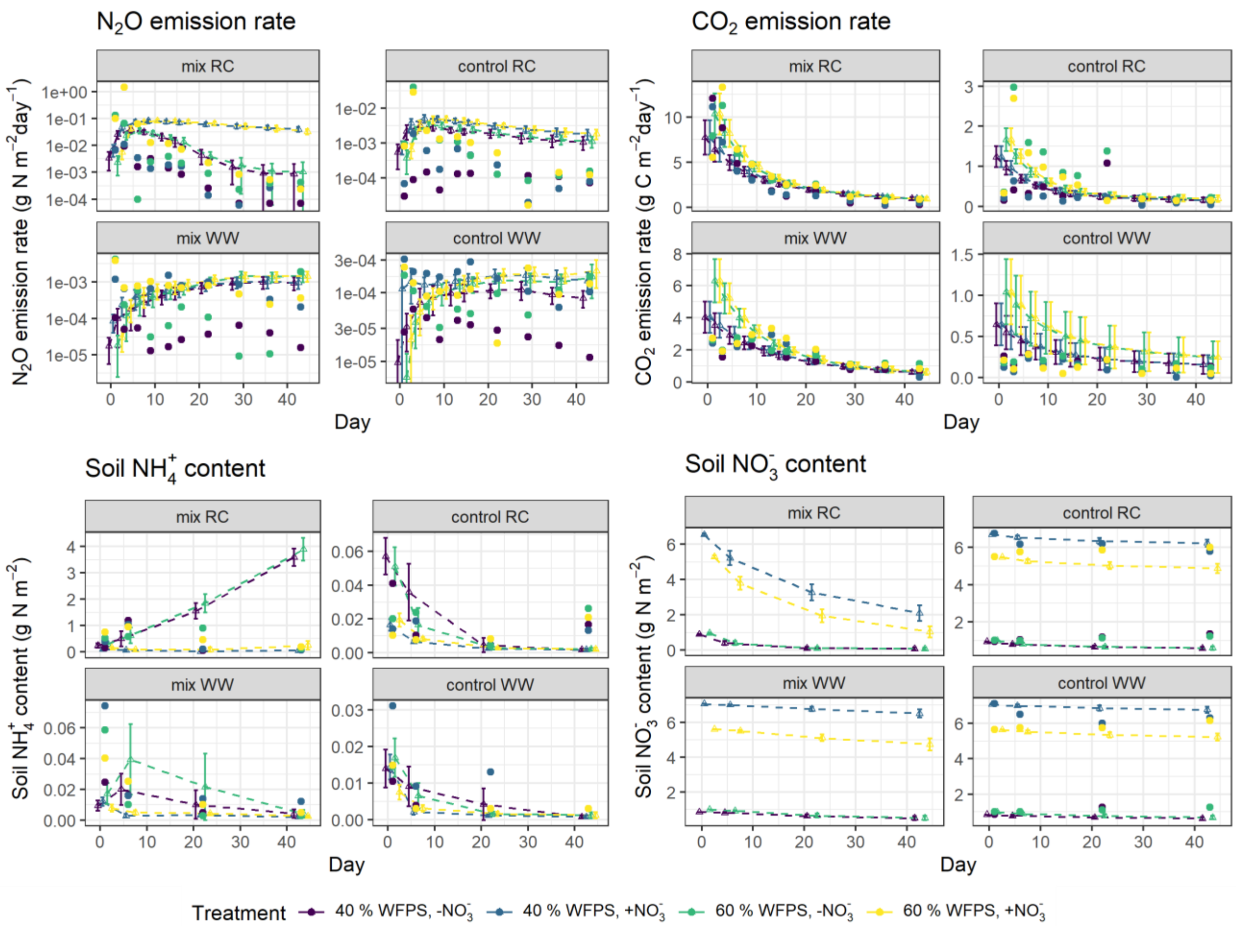


Figure S2: Scatter plots with linear regressions and 95 % uncertainty bands for the residuals of simulated cumulative N_2O fluxes against (a) the observed cumulative N_2O fluxes, (b) the cumulative CO_2 residuals, (c) the average soil NH_4^+ residuals, and (d) the average soil NO_3^- residuals, respectively. Only data from the control treatments were used here.



70 **Figure S3: Simulated and measured daily (a) N_2O fluxes, (b) CO_2 fluxes, (c) soil NH_4^+ content, and (d) soil NO_3^- content during the 43-day incubation. Scatter points represent measured data; and triangles with dashed lines represent simulated data (error bar: 95 % confidence interval). Simulated results were obtained from multi-treatment calibration. Daily measurements presented were re-calculated from the data provided by Taghizadeh-Toosi et al. (2021).**

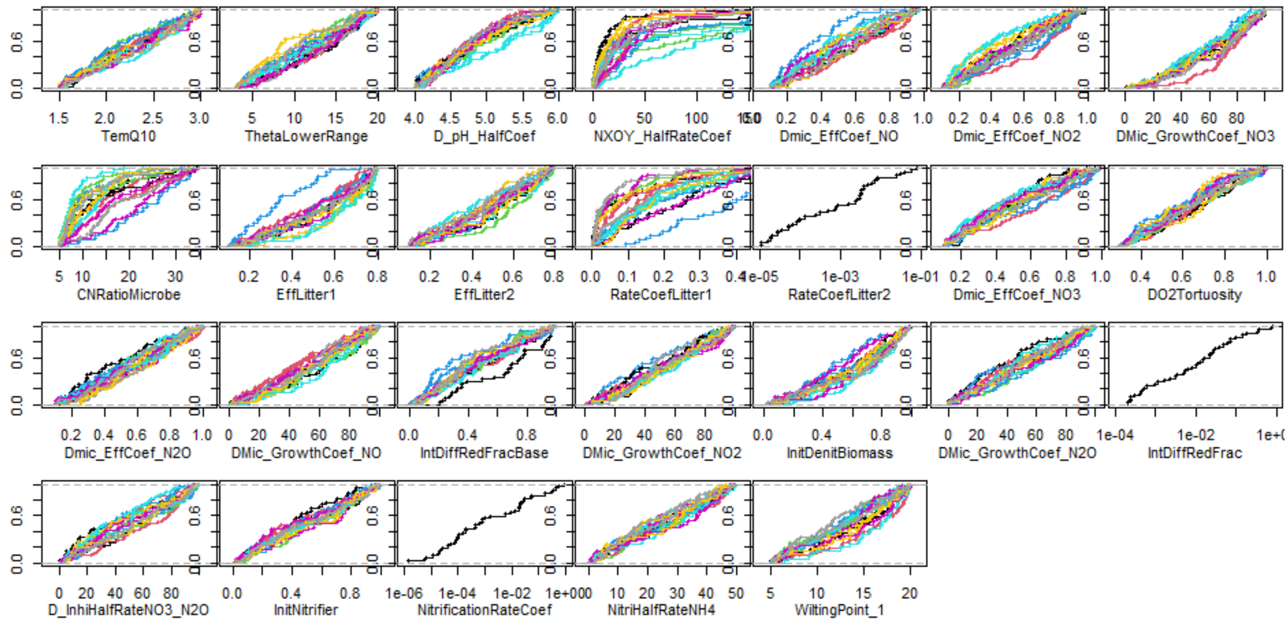


Figure S4: Cumulative distribution frequency of parameter values for accepted runs in all treatments.

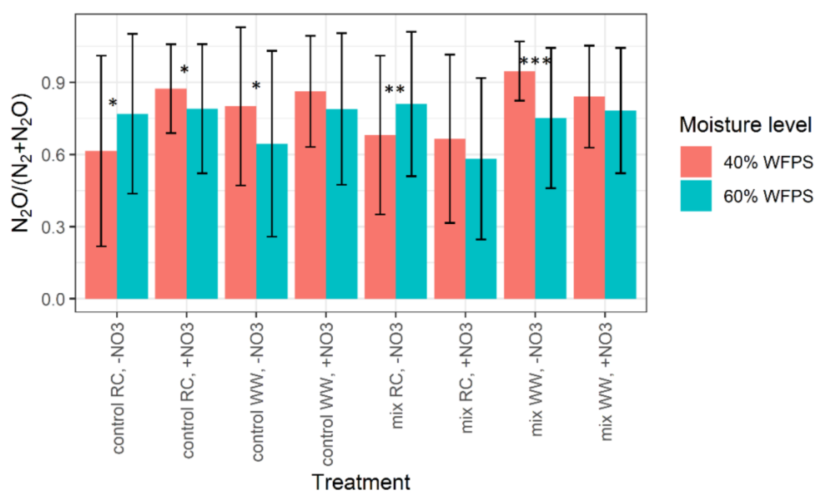


Figure S5: Simulated $N_2O/(N_2O+N_2)$ under two moisture levels across treatments (error bar: standard deviation; * $p < 0.1$, ** $p < 0.05$ and *** $p < 0.01$).

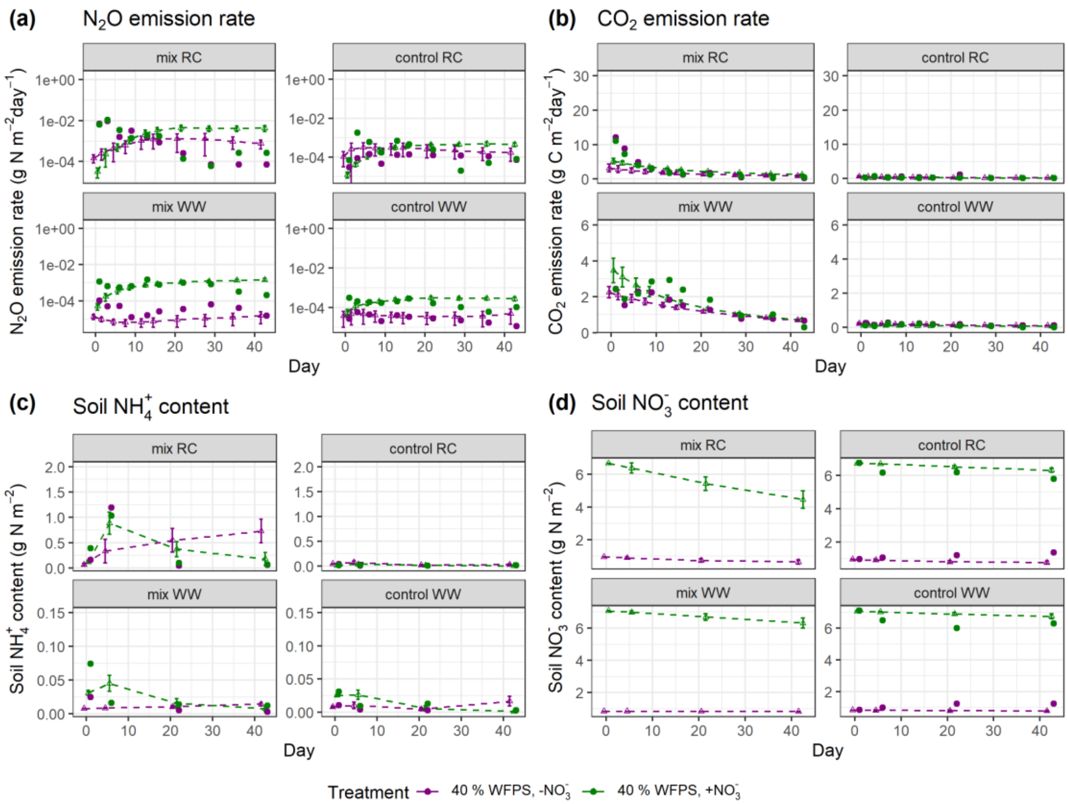


Figure S6: Simulated and measured daily (a) N_2O fluxes, (b) CO_2 fluxes, (c) soil NH_4^+ content, and (d) soil NO_3^- content during the 43-day incubation at 40 % WFPS. Scatter points represent measured data; and triangles with dashed lines represent simulated data (error bar: 95 % confidence interval). Daily measurements presented were re-calculated from the data provided by Taghizadeh-Toosi et al. (2021).

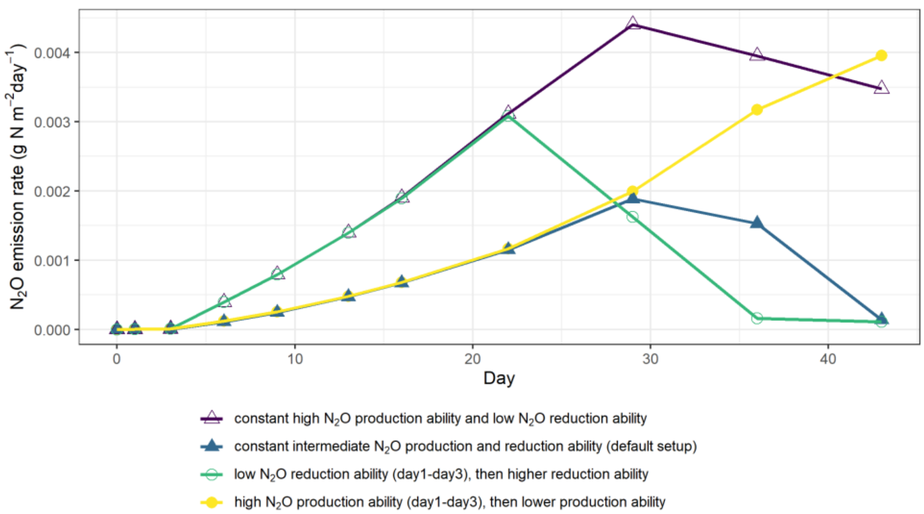


Figure S7: Comparison of simulated N_2O evolution with different d_{effNO} and d_{effN2O} values for treatment 4. The lower $d_{effNxOy}$ values, the higher denitrifiers' ability to reduce N_xO_y. Parameter values in the legend from top to down: 1) fixed values, d_{effNO} = 0.1, d_{effN2O} = 1; 2) fixed values (default), d_{effNO} = 0.428, d_{effN2O} = 0.151; 3) d_{effN2O} = 1 (day 0-day 3) and 0.151 (after day 3), and default d_{effNO}; 4) d_{effNO} = 0.1 (day 0-day 3) and 0.428 (after day 3), and default d_{effN2O}.

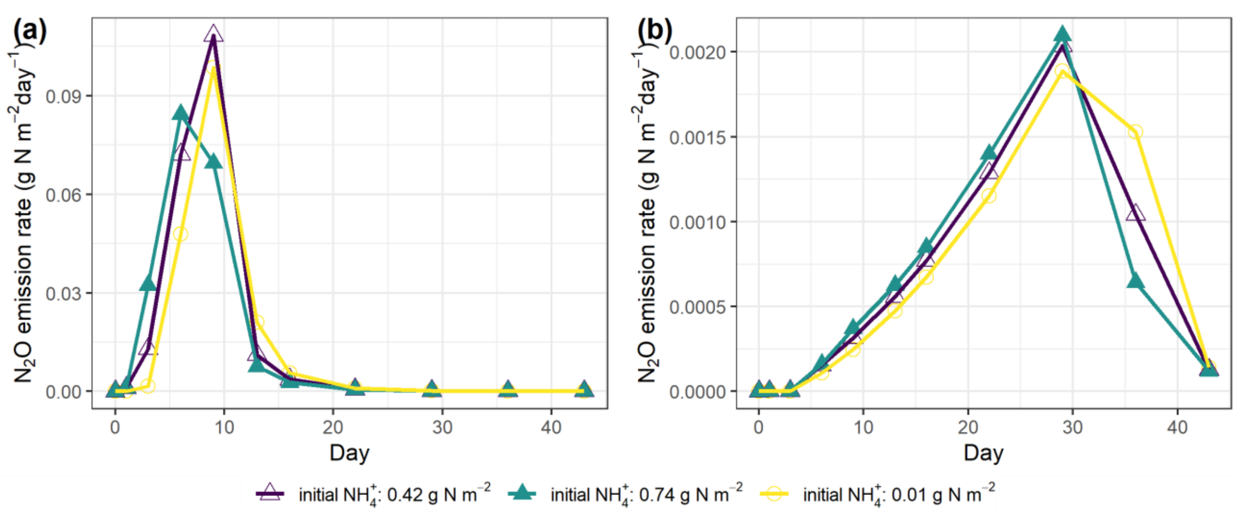


Figure S8: Simulated N_2O evolution with different initial NH_4^+ input values ranging between 0.01 g N m^{-2} (start of experiment) to 0.74 g N m^{-2} (day 1) for treatment 4. Examples of one posterior run with calibrated parameters (a) and one model run with default parameters (b).

Calculating the porosity of soil-residue mixture

The bulk density of soil-residue mixture, $\rho_{b,m}$:

$$\rho_{b,m} = \frac{m_{d,1} + m_{d,2}}{V_{tot,1} + V_{tot,2}}$$

The dry density of soil-residue mixture, $\rho_{d,m}$:

$$\rho_{d,m} = \frac{m_{d,1} + m_{d,2}}{V_{d,1} + V_{d,2}}$$

where $m_{d,i}$ is the dry density (g cm^{-3}), $V_{tot,i}$ is the total volume (cm^3), $V_{d,i}$ is the dry volume (cm^3), and index i in the subscript indicates soil (i = 1) and residue (i = 2).

The mass ratio of soil to residue is a, and $a = m_{d,1}/m_{d,2}$. A bulk soil core with the height of 4 cm contained 5 g of soil per cm^2, and 0.04 g of crop residue was applied into the soil per cm^2. Thus, the calculated a is 125 in the study.

The bulk density of soil-residue mixture, $\rho_{b,m}$, is rewritten as:

$$\rho_{b,m} = \frac{am_{d,2} + m_{d,2}}{\frac{am_{d,2}}{\rho_{b,1}} + \frac{m_{d,2}}{\rho_{b,2}}} = \frac{(a+1)\rho_{b,1}\rho_{b,2}}{a\rho_{b,2} + \rho_{b,1}}$$

The dry density of soil-residue mixture, $\rho_{d,m}$, is rewritten as:

$$\rho_{d,m} = \frac{am_{d,2} + m_{d,2}}{\frac{am_{d,2}}{\rho_{d,1}} + \frac{m_{d,2}}{\rho_{d,2}}} = \frac{(a+1)\rho_{d,1}\rho_{d,2}}{a\rho_{d,2} + \rho_{d,1}}$$

The porosity of the soil-residue mixture, θ_m, was determined by:

$$\theta_m = 100\ \% \times (1 - \frac{\rho_{b,m}}{\rho_{d,m}})$$

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