Table S1. List of important equations for the anaerobic balloon, nitrification, denitrification, and N_2O diffusion.

No.	Equation	Definition	Reference
Anaerobic balloon			
1	$anvf = e^{-SP_{O2} \cdot P_{O2}}$	ANVF expresses the size of the anaerobic balloon	(Smith, 1980, 1990)
2	$D_{soil} = D_{air} \cdot afps^{3.33} / afps_{\max}^{2.0}$	oxygen diffusion coefficient in soil	(Li et al., 2000)
3	$dP_{O2} / dt = (d(D_{soil} \cdot d(P_{O2}) / dz) / dz - R) / afps$	oxygen partial pressure	(Li et al., 2000]
Nitrification			
4	$R_{ngrow} = NMUEMAX \cdot (\frac{[DOC]}{1.0 + [DOC]} + \frac{f(m)}{1.0 + f(m)})$	the relative growth rates of nitrifiers (kg C m-2 d-1)	(Li et al., 2000)
5	$R_{ndeath} = AMAX \cdot (\frac{B_{nit}}{(5.0 + [DOC]) + (1.0 + f(m))})$	the relative mortality rates of nitrifiers (kg C m-2 d-1)	(Li et al., 2000)
6	$B_{nnet} = B_{nit} \cdot (R_{ngrow} - R_{ndeath}) \cdot f(\mathrm{m}) \cdot f(t)$	net increase biomass of nitrifiers	(Blagodatsky and Richter, 1998; Li et al., 2000)
7	$R_{nit} = B_{nit} \cdot \frac{R_{max} \cdot [NH_4]}{(6.18 + [NH_4])} \cdot pH$	nitrification rate (kg N m-2 day-1)	(Norman et al., 2008; Li et al., 2000)
8	$R_{max} = COE_{NR} \cdot N_p$	maximum nitrification rate (day-1)	(Chowdhury et al., 2017)
9	$Np = \min(4 \times 10^8 \cdot CN^{-6.311}, 96.28)$	nitrification potential	(Chowdhury et al., 2017; Lu et al., 2015)
10	$F_{NN2O} = FMAX_{N2O} \cdot R_{nit} \cdot f(t) \cdot f(m)$	maximum N2O fraction during nitrification (kg N m-2 day-1)	(Morkved et al., 2007)
11	$f(t) = [(60.0 - T_{soil}) / 25.78]^{3.503} \cdot e^{[3.503(T_{soil} - 34.22)/25.78]}$	response function of soil temperature	(Li et al., 2000)
12	$f(\mathrm{m}) = \begin{cases} 0.8 + 0.21 \cdot (1.0 - wfps) & wfps > 0.05 \\ 0.0 & wfps < 0.05 \end{cases}$	response function of soil moisture	(Li et al., 2000)
Denitrification			
13	$R_{NOX} = MUE_{NOX} \cdot \frac{[DOC]}{(K_C + [DOC])} \cdot \frac{[DOC]}{(K_N + [NO_X])}$	Relative growth rate of NOX denitrifier	(Li, 2016)
14	$R_{dgrow} = f(t) \cdot (R_{NO3} \cdot f_{NO3}(pH) + R_{NO2} \cdot f_{NO2}(pH) + R_{NO} \cdot f_{NO}(pH) + R_{N2O} \cdot f_{N2O}(pH))$	relative growth rate of total denitrifiers	(Li, 2016)
15	$f_{NO3}(pH) = 1 - 1/(1 + e^{(pH - 4.25)/0.5})$	function of soil pH response to NO_3^-	(Li et al., 2000)
16	$f_{NO2,NO}(pH) = 1 - 1/(1 + e^{pH - 5.25})$	function of soil pH response to NO_2^- and NO consumption rate	(Li et al., 2000)

17	$f_{N2O}(pH) = 1 - 1/(1 + e^{(pH - 6.25)/1.5})$	function of soil pH response to N_2O consumption rate	(Li et al., 2000)
18	$f(t) = 2^{(T_{soil} - 22.5)/10}$	response function of soil temperature	(Li et al., 2000)
Diffusion			
19	$P_{N2O} = D_{N2O} \cdot \frac{\Delta F_{N2O}}{Z_l}$	the diffusion coefficient (kg m-2 h-1)	(Li, 2016)
20	$D_{N2O} = (1.0 - wfps) \cdot (0.018 + 0.124 \cdot C_{clay} + (0.013 - 0.016 \cdot C_{clay}) \cdot 2^{T_{soil}/20} \cdot afps_{max})$	N_2O diffusion coefficient	(Li, 2016)

afps: air-filled porosity; $afps_{max}$: porosity; R: oxygen consumption rate (kg C m^{-2} h^{-1}); Z: soil layer thickness (m); D_{air}: oxygen diffusion coefficient in soil (0.07236 m^{-2} h^{-1}, (Li et al., 2000)); R_{nit}: the nitrification rate (kg N m^{-2} day^{-1}); B_{nit}: biomass concentration of nitrifying bacteria (kg C m^{-3}); $[NH_4]$: NH_4^+ concentration (kg N m^{-2}); pH: soil pH level; R_{max}: maximum nitrification rate (day^{-1}) N_p: the nitrification potential (mg N kg^{-1} day^{-1}); CN: soil C/N ratio; T_{soil}: soil temperature (°C); *wfps*: water-filled porosity; $[DOC]$: dissolved organic carbon concentration (kg m^{-2}); $[NO_X]$: NO_X^- concentration (kg N m^{-2}; i.e. NO_3^-, NO_2^-); R_{NOx}: growth rate of NO_x denitrifiers (h^{-1}); R_{dgrow} : growth rate of total denitrifiers (h^{-1}); ΔF_{N2O}: difference in N_2O flux from two adjacent soil layers (kg N m^{-3} h^{-1}); l: number of layer (from top to bottom) C_{clay}: soil clay concentration

Table S2. Information on the sites used for the model validation.

Region	Lat.	Lon.	Experimental Period	Dominate Crop Type	Fertilizer Rate (kgN ha^{-1} yr^{-1})	Clay	Sand	pH	Soil C:N Ratio	Observed (mgN m^{-2} day^{-1})	Simulated (mgN m^{-2} day^{-1})	Reference
North America	27.0	-109.0	2012-2014	Wheat	260	57.00	22.00	8.00	9.11	0.44	0.34	(Millar et al., 2018)
	45.3	-73.35	2004-2005	Maize, Soybean	160	38.00	23.00	6.30	8.97	1.07	0.93	(Pelster et al., 2011)
	49.7	-112.77	2001-2004	Corn, Wheat, Barely	150	26.00	32.50	7.60	8.41	0.79	0.81	(Ellert and Janzen, 2008)
	46.8	-71.38	2001-2003	Barely	70	22.00	44.00	5.90	15.43	0.34	0.40	(Rochette et al., 2008)
	40.67	-111.15	2004-2005	Wheat	240	8.60	8.80	7.20	9.24	0.36	0.65	(Dusenbury et al., 2008)
	39.75	-83.6	2004-2005	Corn	190	20.00	15.00	7.12	9.08	0.67	0.60	(Ussiri et al., 2009)
	35.5	-119.67	2009-2010	Almond	224	19.30	64.20	7.56	9.03	0.15	0.14	(Schellenberg et al., 2012)
	40.07	-86.93	2004-2006	Corn	250	26.00	43.50	6.00	9.19	1.80	1.72	(Omonode et al., 2011)
	38.56	-121.93	2010-2011	Tomato	237	29.00	43.00	6.35	9.24	0.87	0.85	(Kennedy et al., 2013)
	39.03	-122.05	2009-2010	Almond Orchard	235.5	29.00	43.00	6.35	9.24	0.44	0.70	(Alsina et al., 2013)
	45.15	-73.67	2004-2005	Vegetable	100	23.50	41.00	5.45	17.50	2.69	2.21	(Rochette et al., 2010)
	45.67	-111.15	2004-2006	Wheat	240	8.60	8.80	7.20	8.49	0.18	0.36	(Dusenbury et al., 2008)
	53.42	-113.37	1993-1995	Wheat	100	28.00	33.00	6.50	8.89	0.88	0.83	(Lemke et al., 1999)
	45.92	-66.6	2008-2010	Potato	190	11.00	49.00	6.20	12.70	0.41	0.45	(Snowdon et al., 2013)
	10	-84	1994-1996	Maize Taro	195	22.00	12.00	4.80	9.86	1.91	1.99	(Weitz et al., 2001)
Asia	19.5	109.48	2010-2011	Banana	519	31.00	56.00	5.53	10.00	3.98	2.99	(Zhu et al., 2015)
	18.23	99.05	1997-1998	Maize	46.9	30.00	44.50	4.70	9.72	0.16	0.16	(Watanabe et al., 2000)

	16.48	102.85	1997-1998	Maize	75	56.50	17.00	4.65	8.46	0.13	0.14	(Watanabe et al., 2000)
	14.5	100.85	1996-1997	Maize	62.4	20.50	40.00	7.40	8.76	0.12	0.13	(Watanabe et al., 2000)
	36.05	140.11	1997-1998	Vegetable	400	21.00	37.00	6.15	8.44	0.22	1.33	(Akiyama and Tsuruta, 2002)
	37.02	80.72	2015-2016	Cotton	240	6.00	90.00	8.00	3.41	0.23	0.55	(Kuang et al., 2018)
	36.8	117.9	2011-2012	Wheat, Maize	600	17.10	16.80	8.29	10.00	0.61	0.78	(Shi et al., 2013)
	42.04	116.3	2005-2006	Wormwood	100	15.50	55.00	7.07	10.10	0.68	0.45	(Zhang and Han, 2008)
	23.13	113.25	2013-2014	Corn	360	21.00	31.50	5.20	12.05	0.09	0.14	(唐艺玲 et al., 2015)
	46.8	130.2	2015-2016	Vegetable	770	15.60	31.60	7.60	12.70	1.95	1.72	(Fan et al., 2017)
	34.3	108.03	2015-2016	Vegetable	770	22.70	17.70	7.60	7.00	2.15	2.24	(Fan et al., 2017)
	28.53	113.38	2015-2016	Vegetable	770	12.90	47.10	5.60	6.30	5.33	3.62	(Fan et al., 2017)
	37.6	101.25	2009-2010	Pasture	150	6.00	32.00	8.20	11.00	0.20	0.39	(Zhang et al., 2017)
	24.84	102.81	2005-2006	Vegetable	900	25.00	48.00	6.90	10.55	6.02	3.86	(Guo et al., 2007)
	0.33	102.3	2011-2012	Oil Palm	150	5.00	62.00	4.67	11.00	0.89	0.62	(Sakata et al., 2015)
	1.05	110.87	2010-2012	Oil Palm	113	0.03	97.00	4.78	10.50	0.42	0.27	(Sakata et al., 2015)
	35.63	107.85	2014	Alfalfa	150	22.00	22.00	8.05	7.63	0.28	0.36	(Wang et al., 2018)
	-3.47	114.83	2004-2005	Corn	100	9.60	66.40	4.60	17.20	0.57	0.30	(Hadi et al., 2008)
	17.85	78.48	2010-2011	Sorghum	90	51.50	26.40	8.30	8.50	0.46	0.28	(Ramu et al., 2012)
	23.3	77.4	2012-2013	Wheat, Soybean	110	56.00	15.50	7.85	9.12	0.79	0.64	(Lenka et al., 2017)
	28.67	77.2	2006-2007	Wheat	120	21.00	46.00	8.10	13.70	0.73	0.48	(Bhatia et al., 2010)
	37.2	50.02	2014-2015	Corn	500	22.00	37.00	8.10	8.80	4.00	5.21	(Sadeghi et al., 2018)
Europe	43.67	10.32	2013-2015	Wheat	110	35.00	18.50	7.85	8.62	0.41	0.78	(Volpi et al., 2018)
	43.28	-2.85	2015-2016	Maize, Ryegrass	380	15.00	33.00	7.00	8.00	1.04	0.85	(Huerfano et al., 2018)
	40.53	-3.33	2011-2013	Maize	70	11.50	50.80	7.90	8.09	0.49	0.51	(Tellez-Rio et al., 2017)
	48.85	1.97	2007-2008	Mazie, Wheat	108	31.00	6.50	8.30	12.60	0.63	0.91	(Laville et al., 2011)

	55.96	-2.78	1997	Ryegrass	460	13.00	72.00	7.10	7.77	3.12	3.57	(Smith and Dobbie, 2001)
	55.48	-4.56	1997	Ryegrass	320	33.50	33.50	4.45	9.37	2.28	2.60	(Smith and Dobbie, 2001)
	59.82	10.78	2009-2010	Wheat, Barley	120	21.00	39.00	5.93	10.80	0.80	0.83	(Nadeem et al., 2015)
	60.82	23.47	1993	Barley	103	39.00	20.00	5.80	11.00	0.80	1.79	(Simojoki and Jaakkola, 2000)
	52.86	-6.54	2008-2010	Barley	135	12.50	71.50	7.30	10.00	1.04	1.50	(Abdalla et al., 2014)
	59.55	30.12	2004	Barley, Potato	65	25.50	18.00	5.60	8.83	0.26	0.34	(Balashov et al., 2010)
	55.88	-3.43	1992-1993	Barley, Ryegrass	360	22.00	34.00	5.50	7.77	1.49	1.97	(Clayton et al., 1997)
	51.06	10.82	2011-2013	Poplar Clone, Maize	160	22.00	8.00	7.30	9.60	0.09	0.56	(Walter et al., 2015)
	58.33	13.5	1996-1997	Carrot	100	20.00	43.50	7.20	9.45	4.18	3.75	(Weslien et al., 2012)
	56.49	13	1995-1997	Wheat	120	8.00	35.00	6.80	10.38	0.79	0.82	(Klemedtsson and Smith, 2011)
	58.33	12.65	2005-2006	Wheat	120	20.00	43.50	7.20	6.16	0.30	0.74	
	51.99	5.67	2007-2009	Mazie	110	48.00	20.00	4.80	16.00	1.26	1.12	(Velthof and Mosquera, 2011)
	41.8	1.12	2011-2012	Barley	120	11.80	46.50	8.50	7.18	0.33	1.22	(Plaza-Bonilla et al., 2018)
	47.33	5.03	2012-2013	Wheat	140	41.10	5.30	6.90	11.50	0.89	2.68	(Vermue et al., 2016)
	43.53	-1.505	2010-2013	Legume, Wheat	33	4.00	87.50	7.20	13.24	0.31	0.62	(Peyrard et al., 2016)
Oceanic	-27.43	153.16	2003–2005	Sugarcane,	100	46.00	28.00	5.00	11.88	1.59	1.48	(Allen et al., 2010)
	-35.01	147.33	2013-14	Wheat	100	42.80	37.10	5.60	15.00	0.61	0.55	(Li et al., 2016)
	-27.51	151.78	2010-2011	Corn	270	76.00	6.00	7.30	11.88	0.52	0.36	(Scheer et al., 2016)

	-37.82	142.08	2013-2015	Wheat	0	17.00	71.00	5.60	14.00	0.25	0.23	(Belyaeva et al., 2016)
	-43.67	172.47	2003	Forage	800	20.00	43.00	5.70	11.80	2.89	2.50	(Thomas et al., 2008)
	-31.48	117.2	2009-2010	Wheat	75	8.50	89.00	5.10	7.73	0.02	0.05	(Barton et al., 2013)
South America	-31.5	-63.5	2009–2010	Corn, Soybean	50	17.00	24.00	6.75	8.31	0.54	0.60	(Alvarez et al., 2012)
	-28.25	-52.4	2002-2004	Mazie, Wheat	55	63.00	24.00	5.10	8.87	0.19	0.22	(Jantalia et al., 2008)
	-22.25	-48.57	2010-2011	Surgarcane	60	16.70	62.30	4.30	9.38	0.16	0.16	(do Carmo et al., 2013)
	-22.68	-47.55	2013-2015	Sugarcane,	600	64.80	22.70	5.10	11.88	0.22	0.56	(Lourenco et al., 2019)
Africa	-19.78	47.1	2006-2007	Maize, Soybean	57	30.50	55.50	4.90	10.50	0.15	0.13	(Chapuis-Lardy et al., 2009)
	-17.58	31.23	2000-2002	Maize	0	22.00	73.00	5.10	8.03	0.13	0.11	(Chikowo et al., 2004)
	-17.7	31	2006-2009	Maize	60	11.00	81.00	6.00	8.03	0.19	0.18	(Mapanda et al., 2011)

Fig. S1. Comparison of the variations in the modeled soil NO_3^- content (g N m^{-2}) and the observed soil NO_3^- concentration (mg N kg^{-1}) for the site studied by Wang et al. (2013).

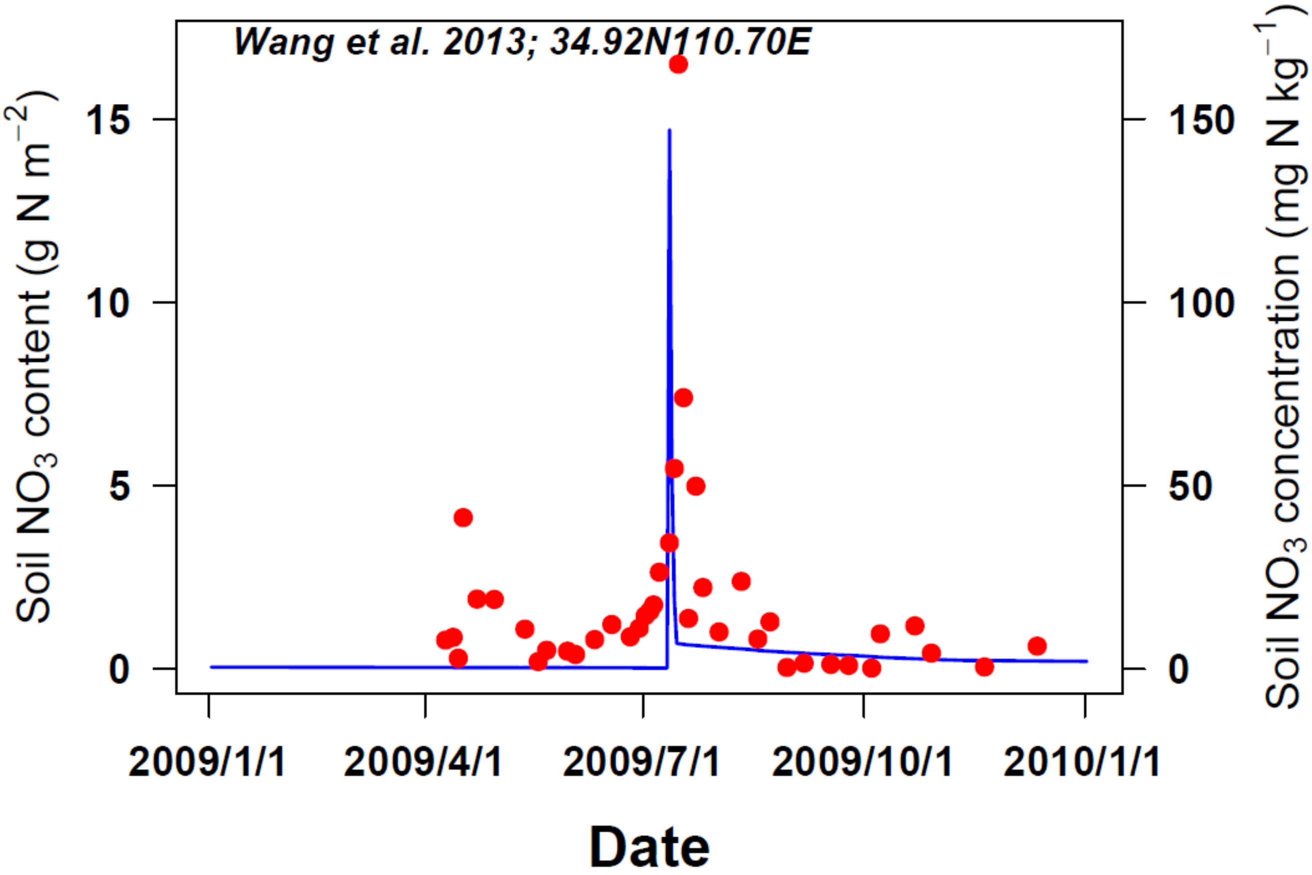
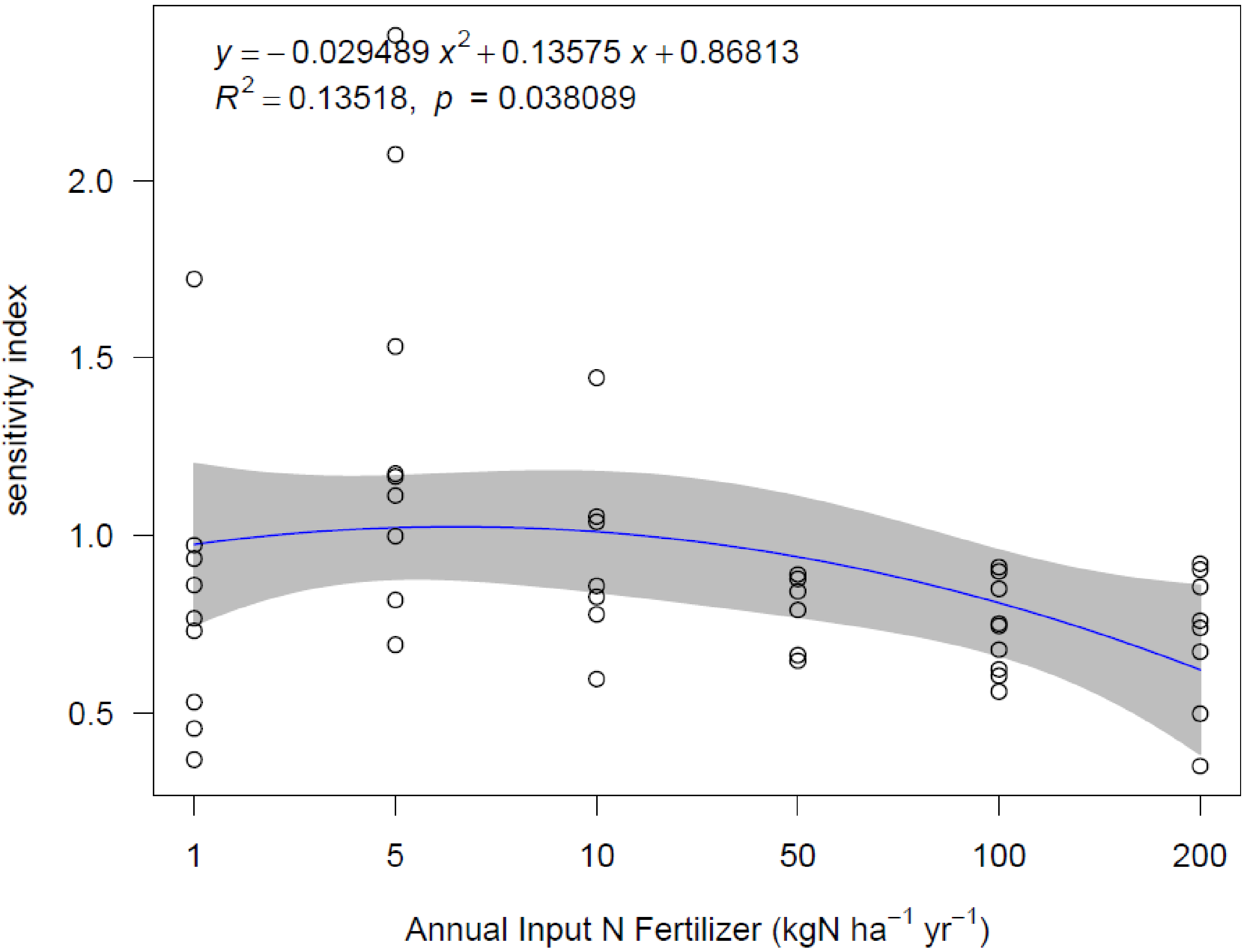


Fig. S2 The variation in sensitivity of the selected parameter COE_{dNO3} with varying chemical fertilizer input. The NH_4^+/NO_3^- ratio was set as 7:1 during the sensitivity analysis, which is a common ratio according to Nishina et al. (2017). The fertilization was set to start in 1961.



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