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Supplement of

Evaluation of denitrification and decomposition from three biogeochemical models using laboratory measurements of N_2, N_2O and CO_2

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Supplementary material

Figures and tables

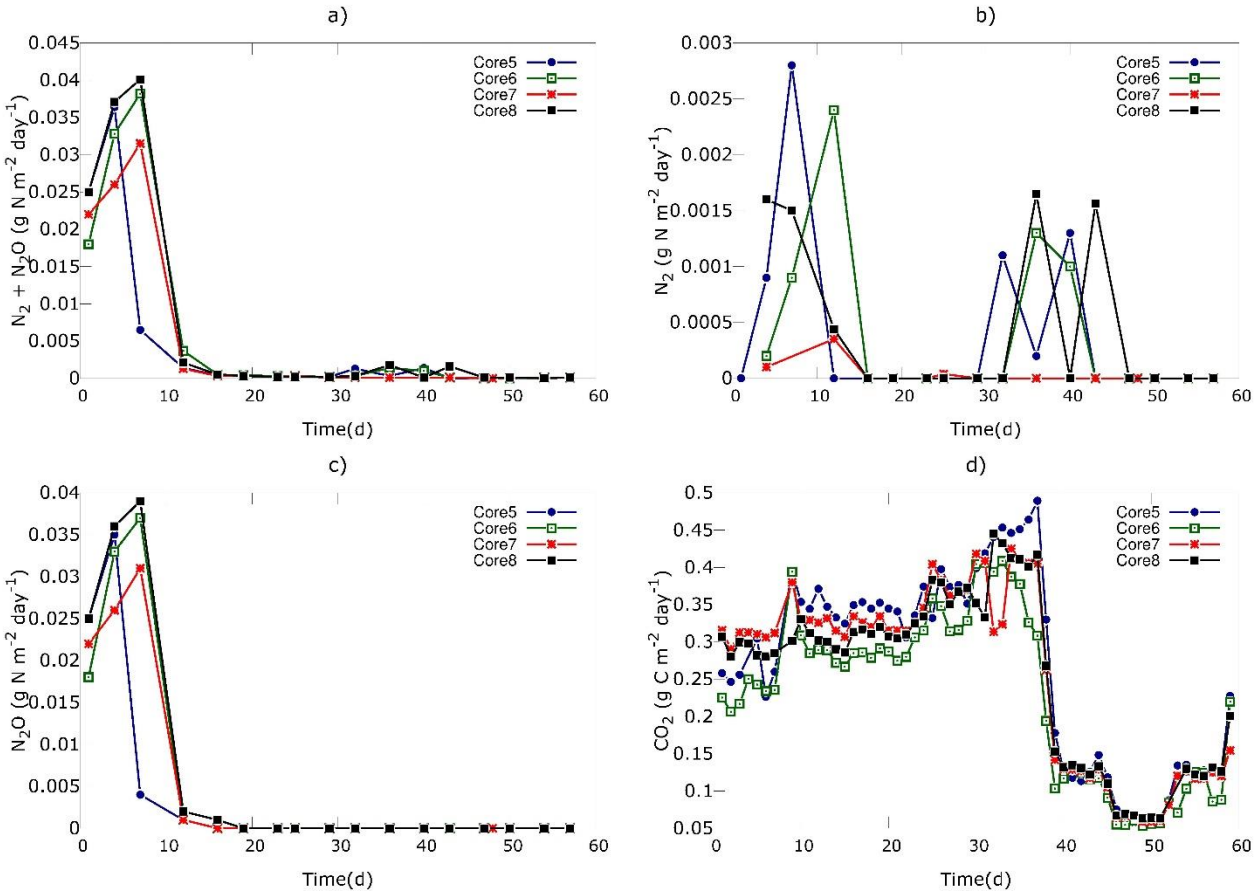

Figure S1 a-d: Measured fluxes of (a) N_2+N_2O, (b) N_2, (c) N_2O and (d) CO_2 throughout a laboratory incubation of a sandy, arable soil from Fuhrberg, Germany. The four re-packed soil cores shown had no ryegrass amendment prior to incubation.

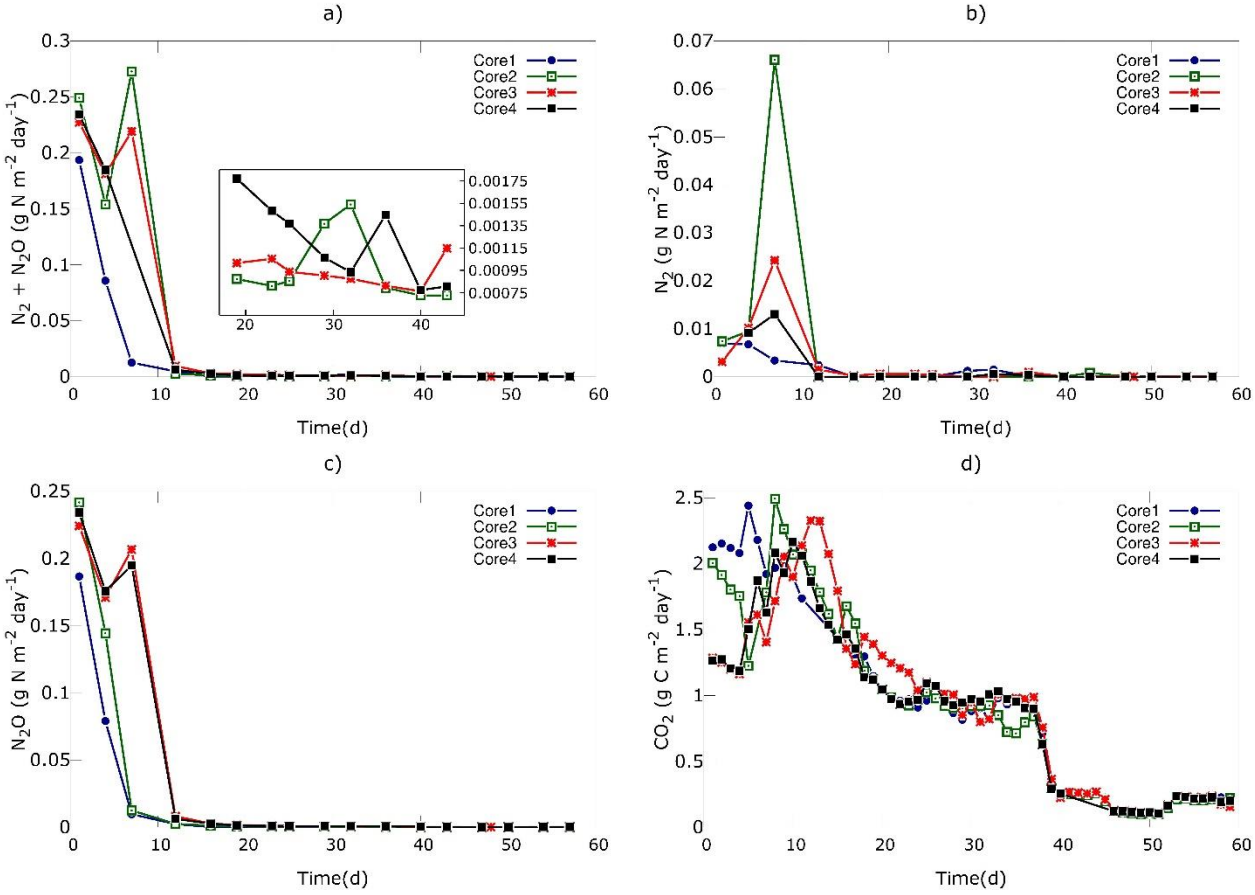

Figure S2 a-d: Measured fluxes of (a) N_2+N_2O, (b) N_2, (c) N_2O and (d) CO_2 throughout a laboratory incubation of a sandy, arable soil from Fuhrberg, Germany. The four re-packed soil cores shown were amended with ryegrass prior to incubation. The nested figure in figure (a) shows the effect of the irrigation and fertilization event on Day 32.

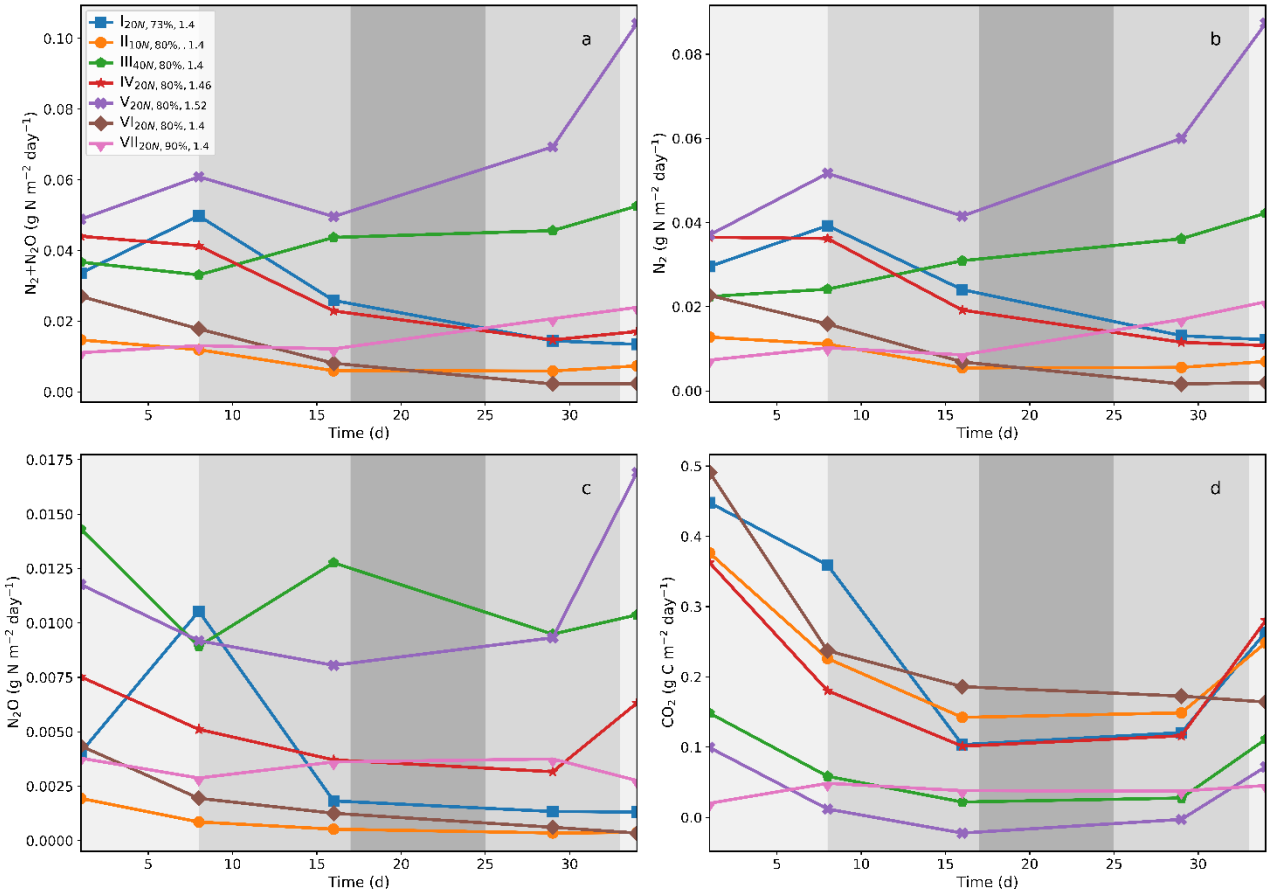

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Figure S3 a-d: Measured fluxes of N_2+N_2O (a), N_2 (b), N_2O (c) and CO_2 (d) of an arable, silt-loam soil from Hattorf, Germany (values shown are the mean of four replicates over a 34 days laboratory incubation). The background colors show the temperature during each time period (light grey: 10°C, middle grey: 6°C, dark grey: 2°C).

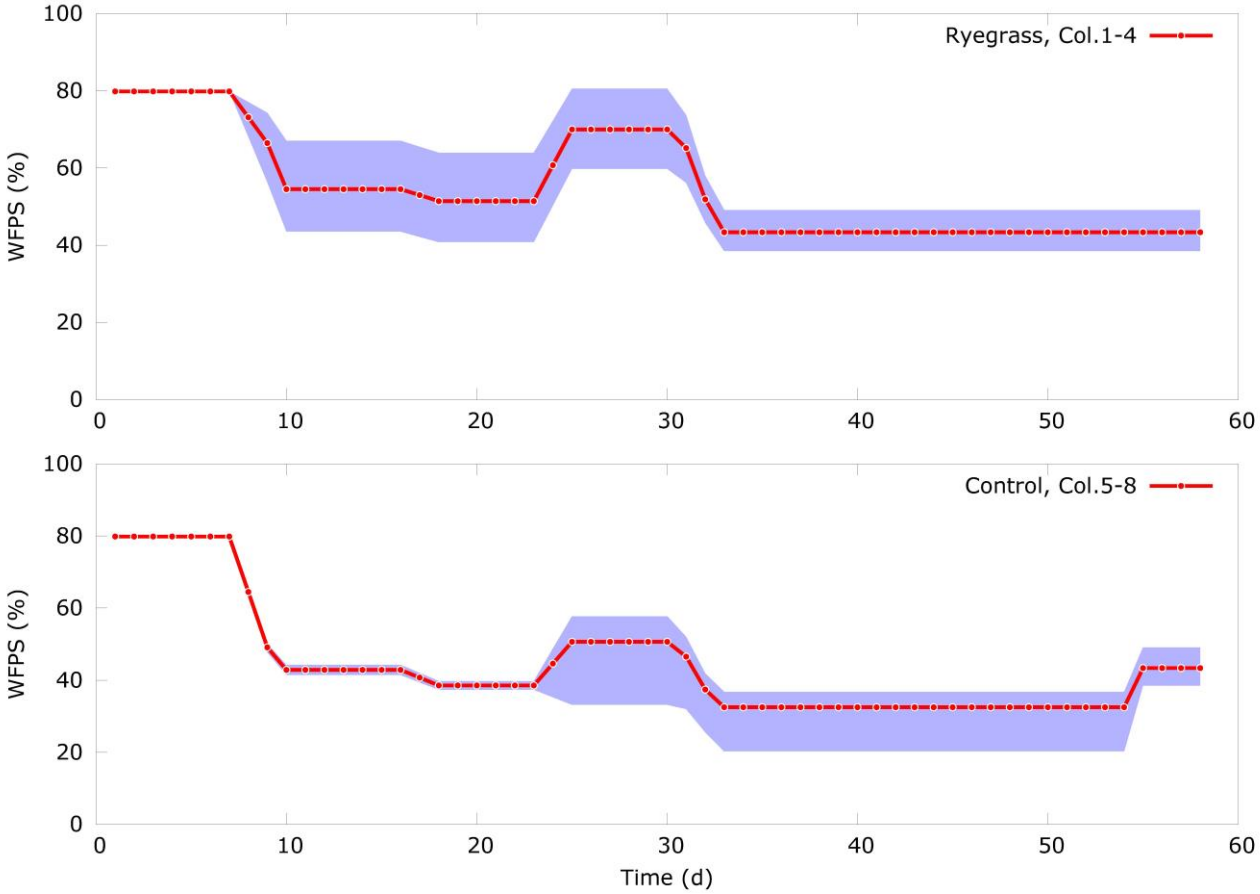

Figure S4: the change in WFPS of eight (2 treatments, 4 parallel columns) re-packed soil columns of a sandy arable soil from Fuhrberg, Germany, over the course of a laboratory incubation. Soil in columns 1-4 had ryegrass incorporated prior to incubation, and Columns 5-8 were without ryegrass. The red line is the mean value, and the blue areas are the SD.

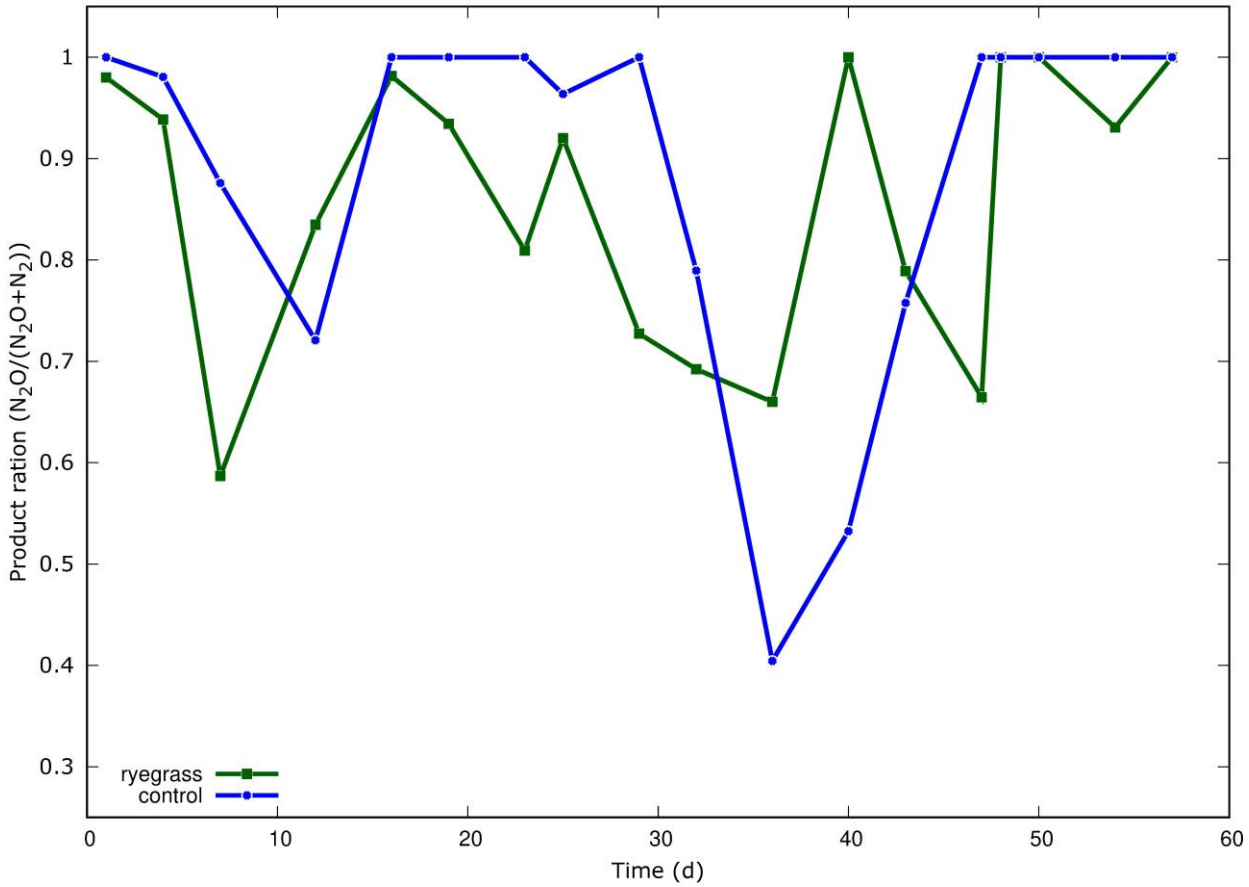

Figure S5: the $N_2O/(N_2+N_2O)$ product ratio throughout a laboratory incubation of a sandy arable soil from Fuhrberg, Germany. Data shown is the average of four replicate re-packed soil cores for each treatment (i.e. with ryegrass amendment or control).

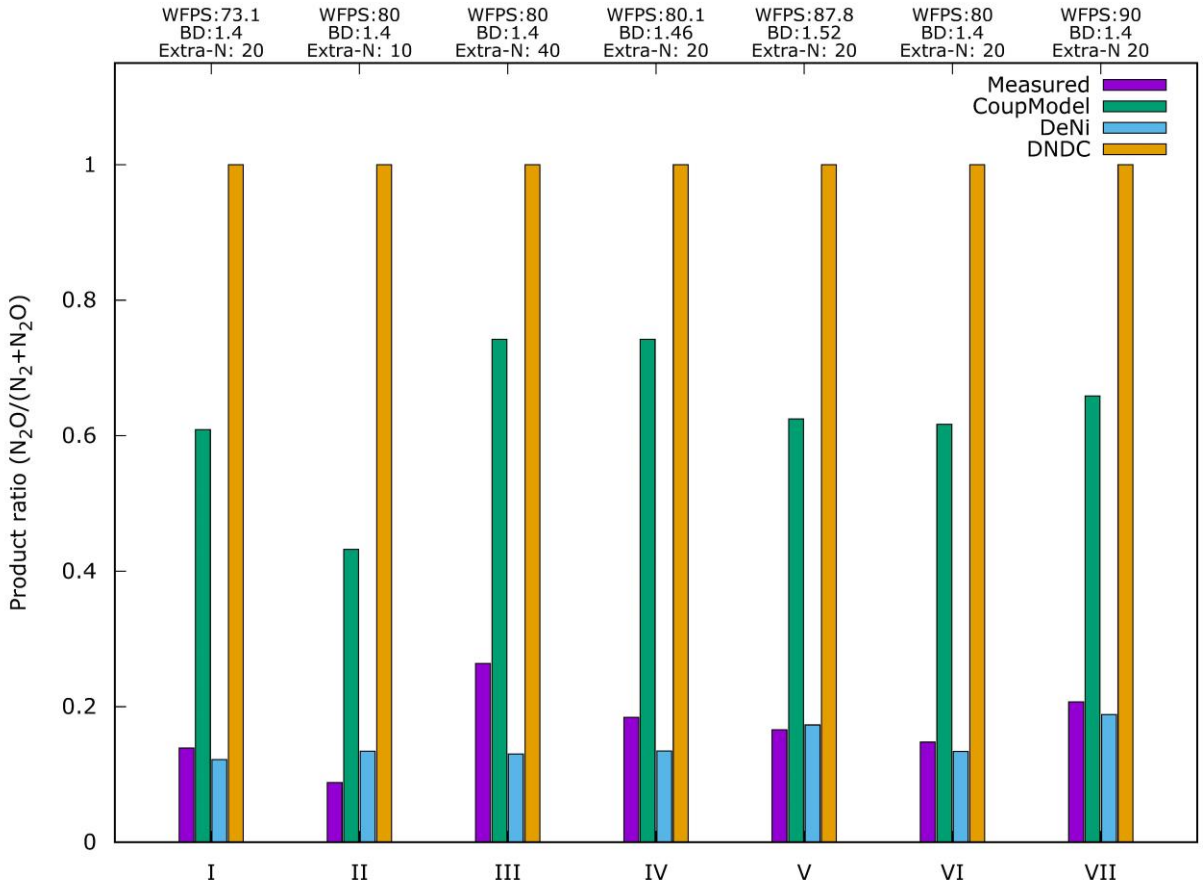

Figure S6: the $N_2O/(N_2+N_2O)$ ratio of flux measurements during a laboratory incubation of arable, silt-loam arable soil from Hattorf, Germany, compared with modeled fluxes using three biogeochemical models: Coup, DeNi and DNDC.

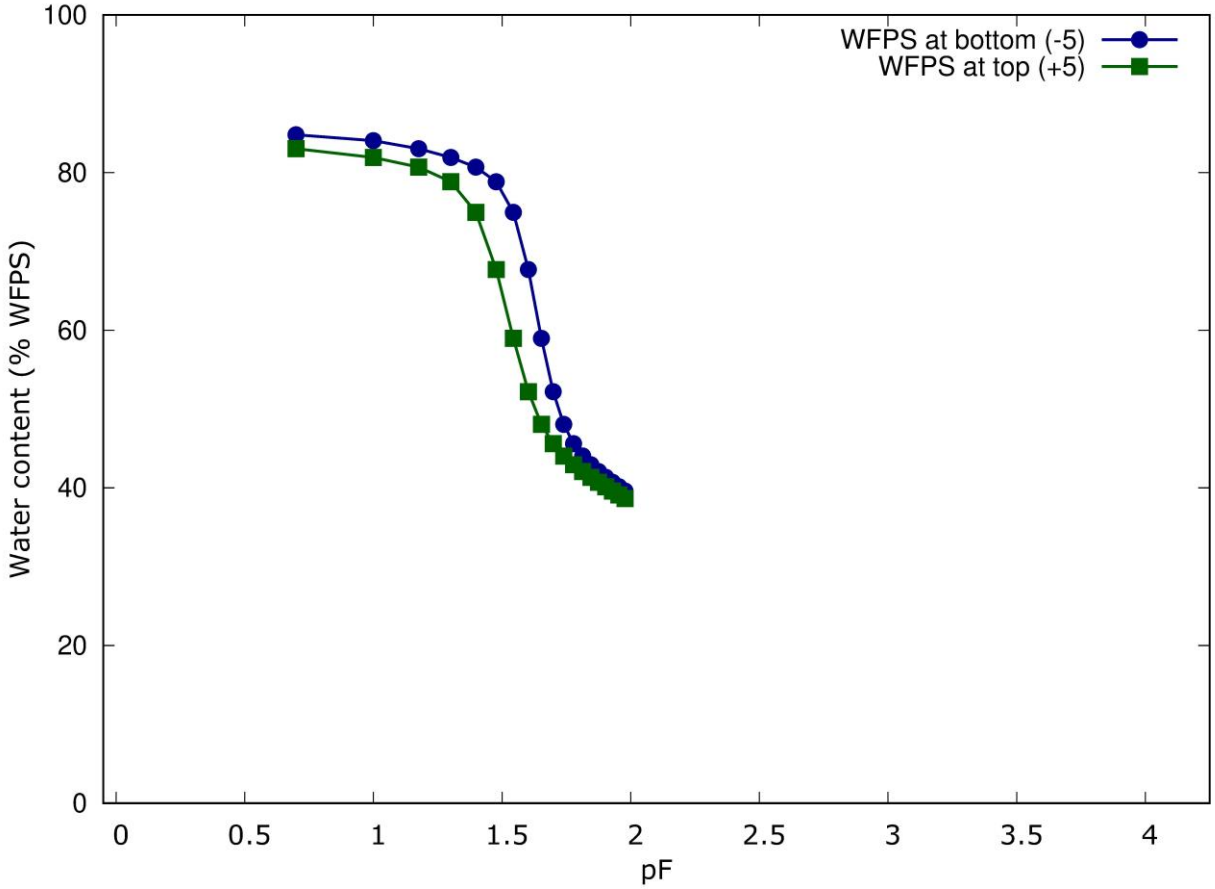

Figure S7: water retention curve of a sandy arable soil from Fuhrberg, Germany, showing WFPS for the upper and lower boundary of the soil core in relation to pressure head (shown as pF = log (-cm H_2O) as calculated from core height assuming equilibrium conditions).

Table S1: Experimental settings during a 5-8 week laboratory incubation of re-packed soil cores from Fuhrberg, Germany (sand) and Hattorf, Germany (silt-loam)

Soil	Week of Experiment	1	2	3	4	5	6	7	8
Sand	Bottom water potential [kPa]	-10	-20	-60	-60	-10	-10	-10	-10
	Temperature [°C]	20	20	20	20	20	10	5	10
	Irrigation with water [mm]	-	-	-	-	10	-	-	-
	Irrigation with NO_3^-solution [mm / mg N kg^{-1}]	-	-	-	-	30 / 30	-	-	-
Silt-loam	Temperature [°C]	10	6	2	6	10	-	-	-

Table S2: The settings of the CoupModel – Switches

Modules	Processes	Name	Options
Abiotic driving variable	Forcing Biological conditions	SoilWaterFlowInput	Simulated
External N Inputs		N fertilization	Parameters
		N irrigation	on
Gas Processes	Initial NC Conditions	Trace Gas Emission	Direct loss
Model structure	Heat	HeatEq	off
	Organic	Nitrogen and Carbon	Abiotic driving variables
	General	NitrogenCarbonStep	Independent
		OnlyNC	Yes
Soil Hydraulic	Storage	Hydraulic Function	Genuchten
	Water	Pedo Function	Texture parameters
Soil mineral N Processes	Initial NC Conditions	Denit Depth Distrib.	Constant
	Denitrification	Denitrification	Microbial based
	Initial NC Conditions	Initial Nitrifier	Constant
	Nitrification	Nitrification	Microbial based
Soil Organic Processes	Transport	Dissolved Organic	On

Table S3: The settings of the CoupModel – Parameters

Modules	Process		Name	Value
Abiotic driving variable	Forcing Conditions	Biological	Soil Temperature	20 °C
			Soil Water Content	34.65 Vol.%
Extra N inputs	Forcing Conditions	Biological	N Fert Dis k	0.001
			N Fert NH_4 Frac	0
Soil Mineral N Processes	Denitrification		DMic_GrowthCoef_N_2O	100 /day
			DMic_GrowthCoef_NO	100 /day
			D_InhiHalfRateNO_3_N_2O	50 mg/l
			D_PH_HalfCoef	4.25
			D_PH_ShapeCoef	0.5
			DeNiActivityRateCoef	1 /day
			DenitNitrateHalfSat	5
			Dmic_EffCoef_N_2O	0.1
			Dmic_EffCoef_NO	0.151
			Dmic_RespCoef_N_2O	100 /day
			Dmic_RespCoef_NO	20 /day
	Initial NC Conditions		InitDenitBiomass	2 gN/m^2
	Denitrification		NxOy_Doc_HalfRateCoef	5 mg/l
			NxOy_HalfRateCoef	10 mg/l
Soil Organic Processes	Decomposation		Eff Litter1	0.3
			Eff humus	0.3
	Initial NC Conditions		Init H CN Tot	10
			Init H Depth	-0.3 m
			Init H NTot	213.82 g/m^2

	Decomposation	Init L1 CN Tot	15.1
		Init L1 Depth	-0.3 m
		Init L1 NTot	20 g/m^2
		RateCoefHumus	0.00041 /day
		RateCoefHumusDis	0.0001 /day
		RateCoefLitter1	0.02 /day
		RateCoefLitter1Dis	0.0005 /day

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Table S4: The settings and capability of the CoupModel, DeNi and DNDC

	CoupModel	DeNi	DNDC
Run time	Daily/hourly	Daily	Daily
NO_3^-	+	+	+
NH_4^+	+	+	+
C pools	+	-	+
N pools	+	-	+
C/N ratio	+	-	+
Daily water data	+	+	-
Water retention curve	+	-	-
Soil specific water data	-	+	+
Decomposition	First order kinetic	$S_{CO2} = S_{max}\ S_{WFPS}\ S_{SoilTemp}$	First order kinetic
Nitrification	nitrifying microbes are simulated explicitely or not explicitely	empirical function taking NH_4^+, WFPS, pH and respiration into account	nitrifying microbes are simulated explicitely
Denitrification	Denitrifiers are simulated explicitly; considering mineral N, WFPS, C_{org}, CO_2 and soil depth	empirical function taking NO_3^-, WFPS and respiration into account	Denitrifiers are simulated explicitly

Table S5. the effect of the water manipulation (Table S5.; suction or irrigation) on the NO_3^- content (4 replicates of 2 treatments: C1-4 with and C5-8 without ryegrass) of a sandy arable soil from Fuhrberg, Germany. The table shows the decrease or increase of the NO_3^- concentration of the soils between the treatment events according to the removed or added water. The values were estimated from the NO_3^- concentration of the leachate or added water.

Days	Core 1	Core 2	Core 3	Core 4	Core 5	Core 6	Core 7	Core 8
	NO_3^- (mg N kg^{-1})							
8	-7.37	-13.54	-0.67	-5.82	-22.31	-33.84	-33.39	-33.56
9	-7.93	-9.64	-0.94	-1.84	-2.89	-5.61	-6.42	-5.09
17	-2.07	-1.00	-0.14	-0.10	-1.73	-3.87	-3.73	-4.36
24	-2.04	-1.10	-0.07	-0.03	-6.72	-2.06	-3.04	-3.49
29	-23.31	-13.89	-4.55	-0.47	-3.95	-8.66	-14.03	-11.86
31	-24.13	-28.69	-17.14	-20.79	-27.02	-25.64	-36.19	-29.18
32	14.66	14.66	14.66	14.66	14.66	14.66	14.66	14.66

Table S6. water manipulation (irrigation water or leachate, extra NO_3^-) data of the 1-4 ryegrass treated and 5-8 control columns of for a laboratory incubation of sandy arable soil from Fuhrberg, Germany

Days	Leaching water (ml)								Added water (ml)	Extra KNO_3 mg NO_3^-/ dm^3
	Core 1	Core 2	Core 3	Core 4	Core 5	Core 6	Core 7	Core 8	Core 1-8	Core 1-8
5	0	0	0	0	101.93	0	0	0	-	-
9	55	120	39	167	229	220	210	214	-	-
17	68	128	52	90	44	45	49	39	-	-
23	24	22	23	19	28	34	28	32	-	-
25	24	22	23	19	193	28	34	28	-	-
29	-	-	-	-	-	-	-	-	162.9	-
31	246	239	228	231	216	254	236	222	488.7	30
32	533	564	519	523	542	531	524	574	-	-
58	154	105	126	96	75	64	72	69	-	-

Table S7: Averages and standard deviation (n=4) of measured cumulative fluxes (N_2, N_2O, N_2+N_2O: g N m^{-2} day^{-1}; CO_2: g C m^{-2} day^{-1}) and $N_2O/(N_2+N_2O)$ ratio of cumulated fluxes (dimensionless) from two laboratory incuations: arable, silt-loam soil from Hattorf, Germany (34 days; 7 treatments) and arable, sandy soil from Fuhrberg, Germany (58 days; 2 treatments). Shown in the treatment column are added NO_3^- (10/20/40 mg KNO_3-N / kg dry soil), water-filled pore space (WFPS; 73-90%) and bulk density (BD; 1.4-1.52 g cm^{-3}) for the silt-loam soil. Superscript letters indicate significant differences within sites, between treatments ($p<0.05$; Tukey HSD for silt-loam and Wilcoxen for sand).

	Treatment		N_2	N_2O	N_2+N_2O	$N_2O/(N_2+N_2O)$	CO_2
I	N: 20 WFPS: 73 BD: 1.4	Silt-loam soil	0.118±0.133	0.019±0.022	0.137^{c}±0.140	0.139	1.295^{a} ±0.715
II	N: 10 WFPS: 80 BD: 1.4		0.042±0.026	0.004±0.002	0.046^{c}±0.025	0.088	1.142^{a}±0.273
III	N: 40 WFPS: 80 BD: 1.4		0.156±0.116	0.056±0.025	0.212^{ab}±0.137	0.264	0.368^{bc}±0.515
IV	N: 40 WFPS: 80 BD: 1.46		0.114±0.107	0.026±0.025	0.140^{bc}±0.131	0.184	1.041^{ab}±0.434
V	N: 20 WFPS: 88 BD: 1.52		0.278±0.124	0.055±0.016	0.333^{a}±0.138	0.166	0.158^{c}±0.212

	N: 20						
VI	WFPS: 80		0.049±0.049	0.009±0.011	0.058^{c}±0.059	0.148	1.251^{a}±0.503
	BD: 1.4						
	N: 20						
VII	WFPS: 90		0.064±0.049	0.017±0.009	0.081^{bc}±0.051	0.207	0.190^{c}±0.316
	BD: 1.4						
C1-4	Added ryegrass	Sandy soil	0.490±0.075	4.82±0.632	5.31^{a}±0.677	0.908	52.7^{a}±9.74
C5-8	Control		0.053±0.005	0.638±0.097	0.691^{b}±0.100	0.924	15.2^{b}±2.06

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