Supplementary material

Figures and tables

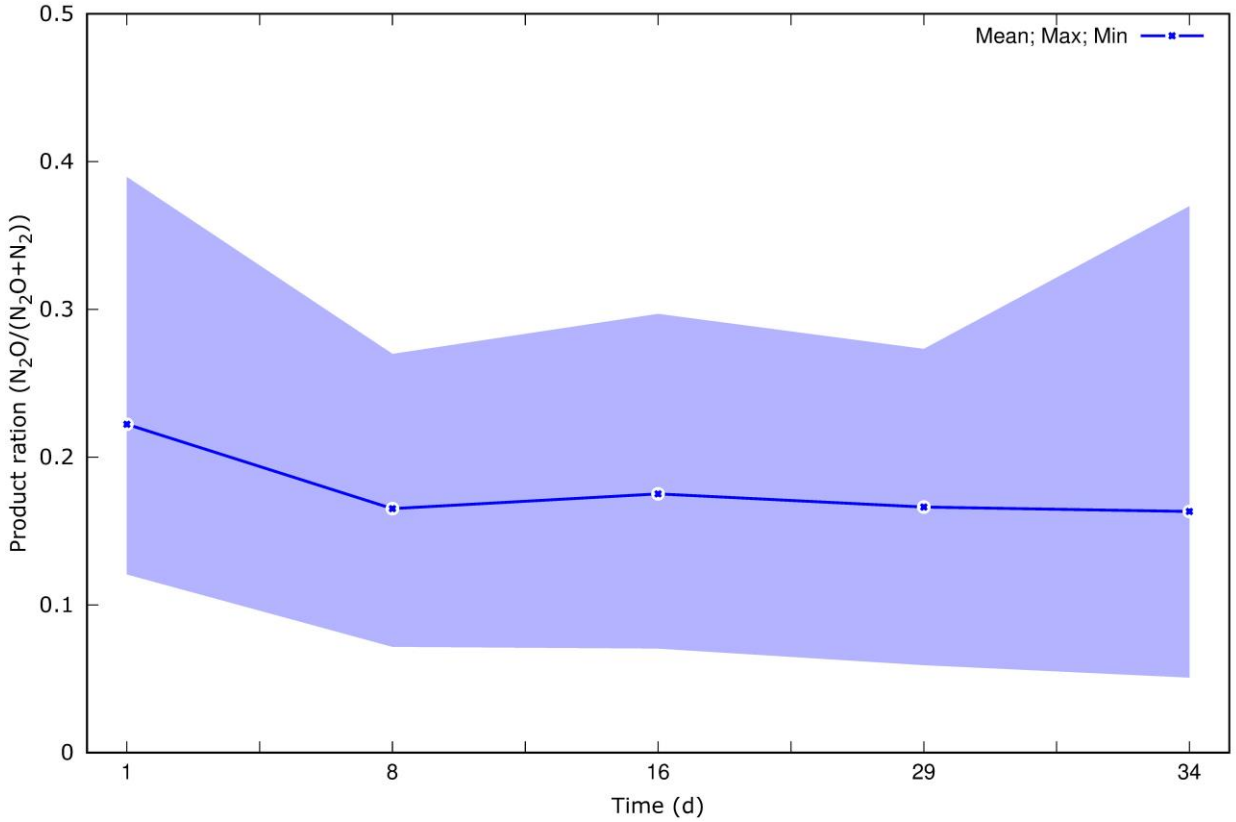

Figure S.1: average, maximum and minimum $N_2O/(N_2 + N_2O)$ product ratio of seven treatments of a silt-loam arable soil from Hattorf, Germany

Table S.1. 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

	Leaching water (ml)								Added water (ml)	Extra KNO_3
Days										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 S.2. the effect of the water manipulation (Table S.1.; 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 S.3: $N_2O/(N_2+N_2O)$ ratio of the measured and modeled results of a sandy arable soil from Fuhrberg, Germany

	Measured	DeNi	CoupModel	DNDC

Core 1	0.934	0.393	0.336	1
Core 2	0.954	0.380	0.308	1
Core 3	0.881	0.432	0.345	1
Core 4	0.945	0.417	0.307	1
Core 5	0.889	0.338	0.319	0.9999
Core 6	0.928	0.350	0.310	0.9999
Core 7	0.992	0.350	0.308	0.9999
Core 8	0.921	0.353	0.307	0.9999

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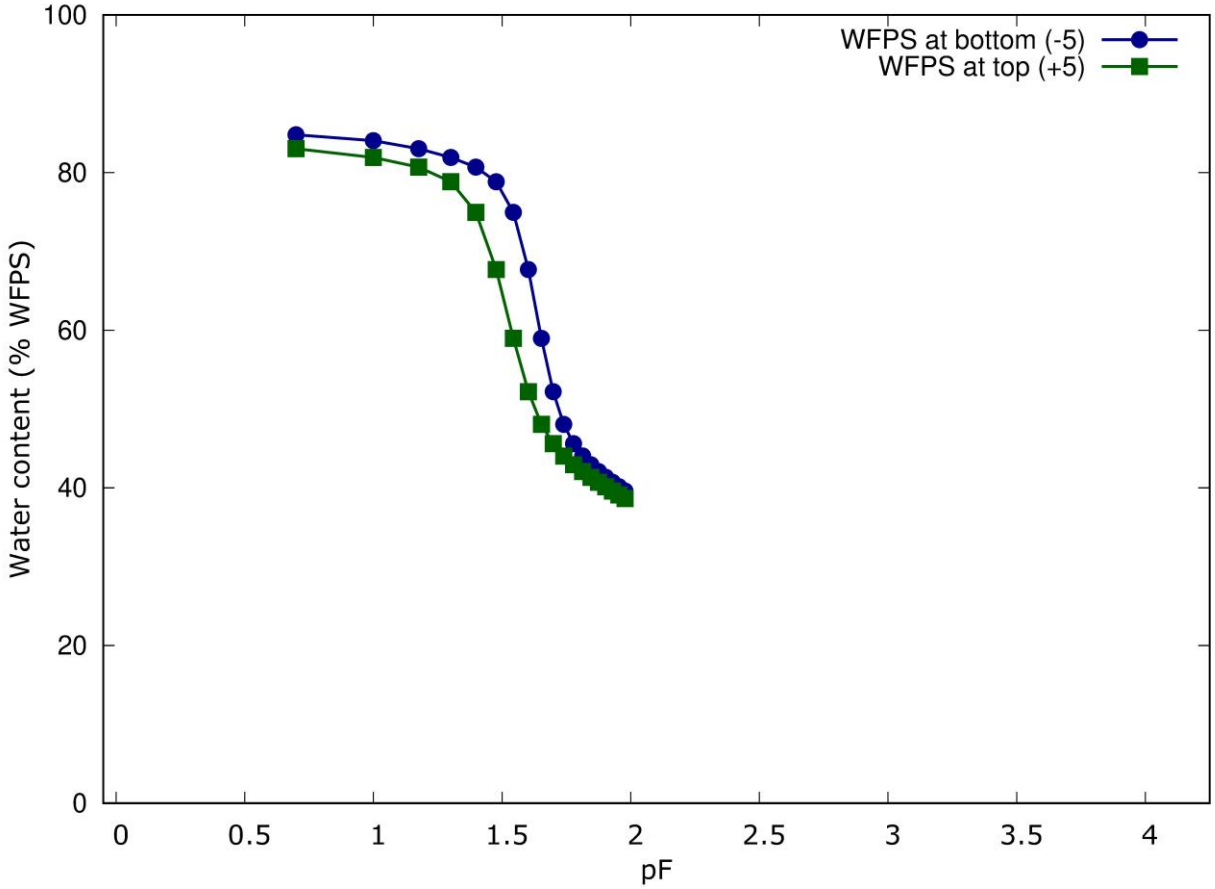

Figure S.2: water retention curve of a sandy arable soil from Fuhrberg, Germany, showing WFPS for the upper and lower boundary of the soil core in relation to pressure head (shown as pF = log (-cm H_2O) as calculated from core height assuming equilibrium conditions).

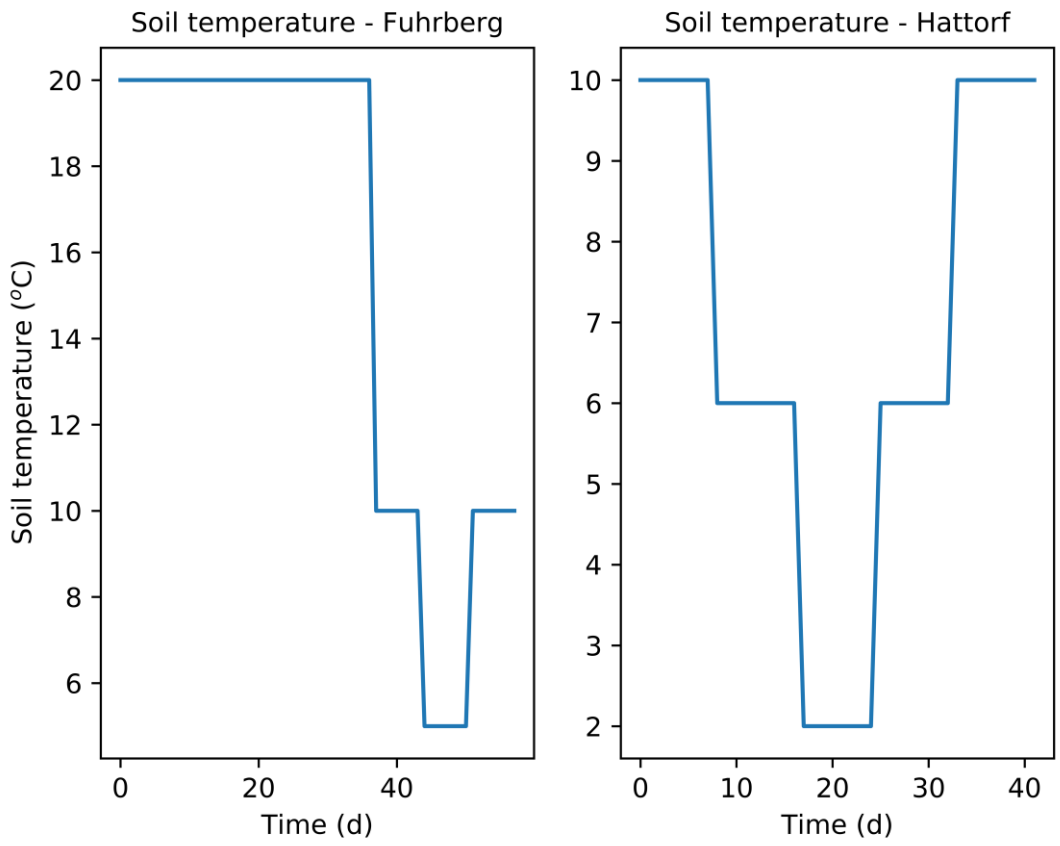

Figure S.3: soil temperature manipulation over the course of two laboratory incubations of repacked sandy arable soil from Fuhrberg, Germany (58 days, 20°C, 10°C, 2°C, 10°C) and silt-loam arable soil from Hattorf, Germany (34 days, 10°C, 6°C, 2°C, 6°C, 10°C).

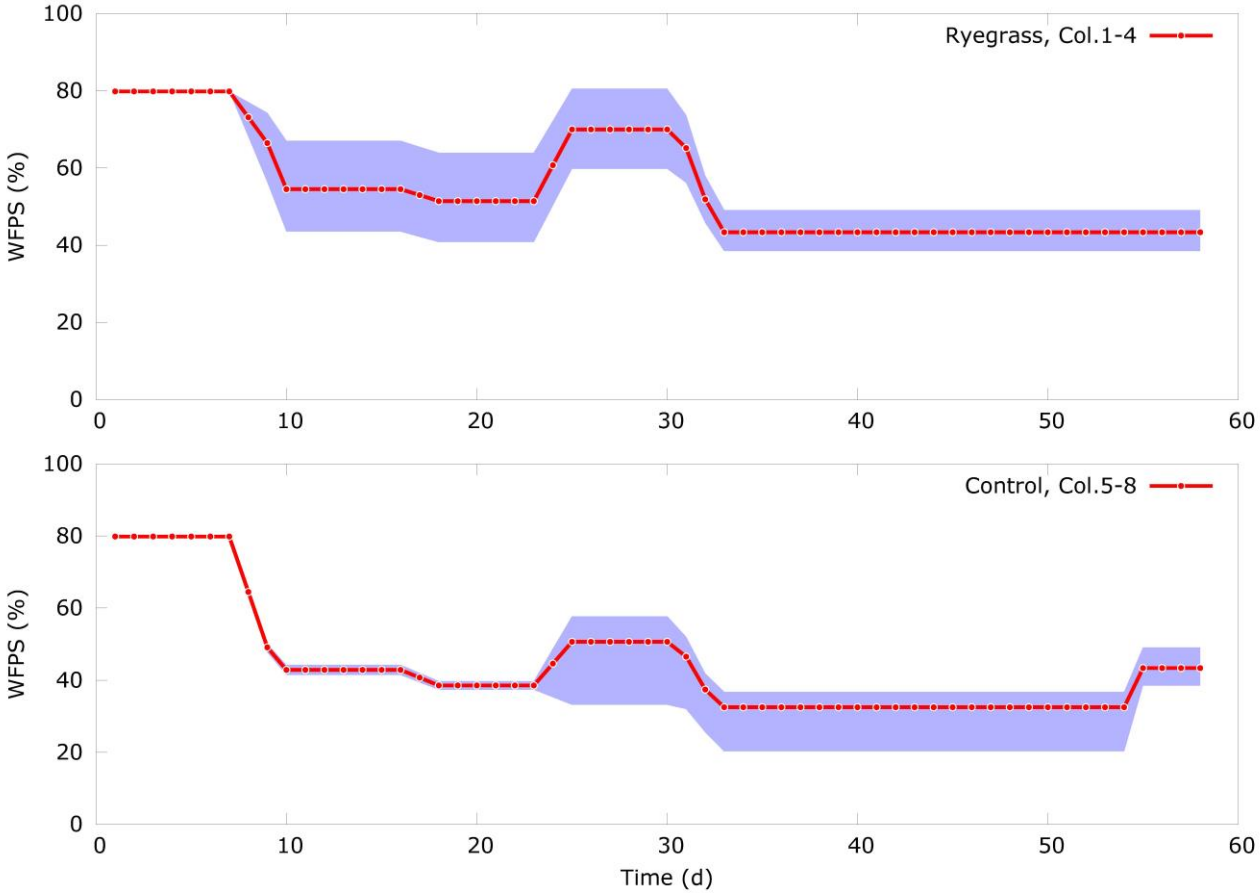

Figure S.4: the change in WFPS of eight (2 treatments, 4 parallel columns) re-packed soil columns of a sandy arable soil from Fuhrberg, Germany, over the course of a laboratory incubation. Soil in columns 1-4 had ryegrass incorporated prior to incubation, and Columns 5-8 were without ryegrass.

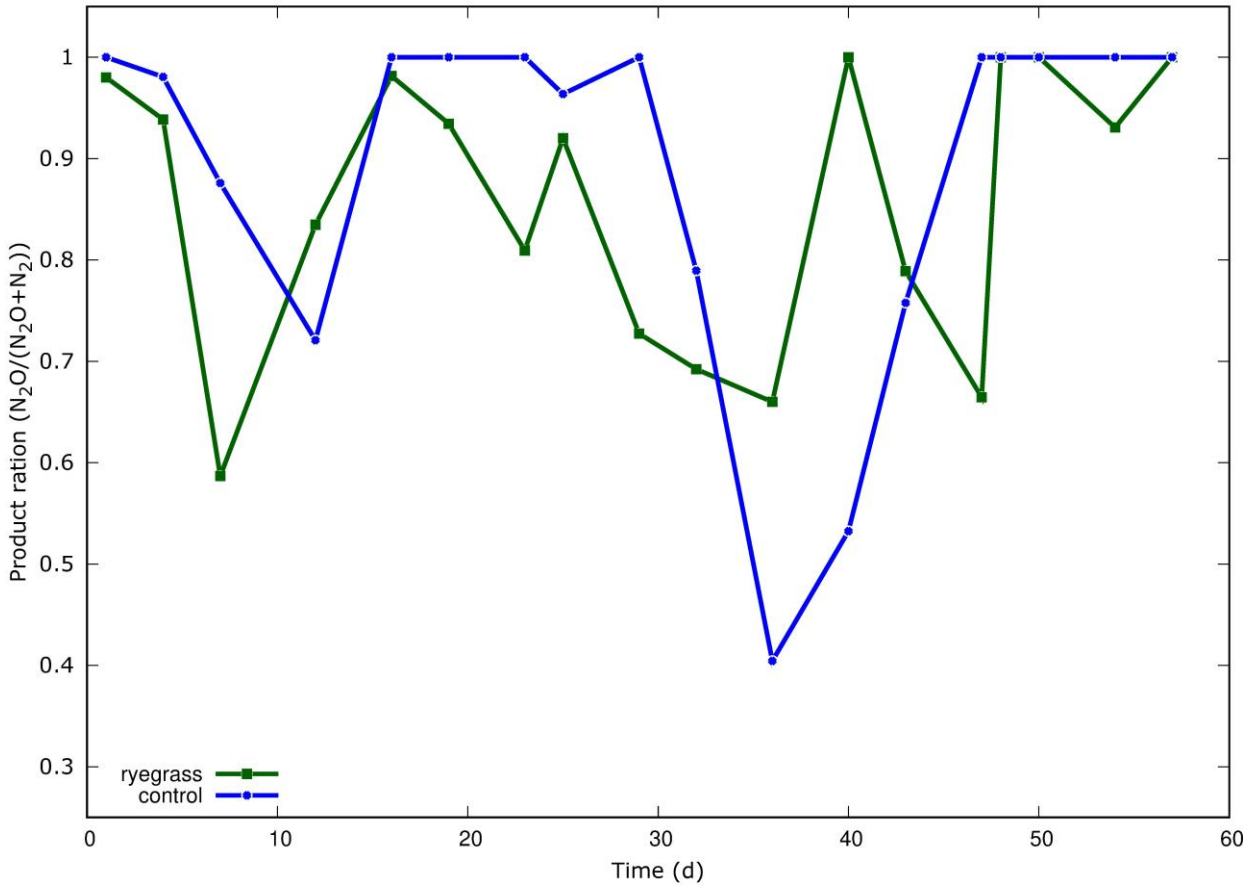

Figure S.5: the $N_2O/(N_2+N_2O)$ product ratio throughout a laboratory incubation of a sandy arable soil from Fuhrberg, Germany. Data shown is the average of four replicate re-packed soil cores for each treatment (i.e. with ryegrass amendment or control).

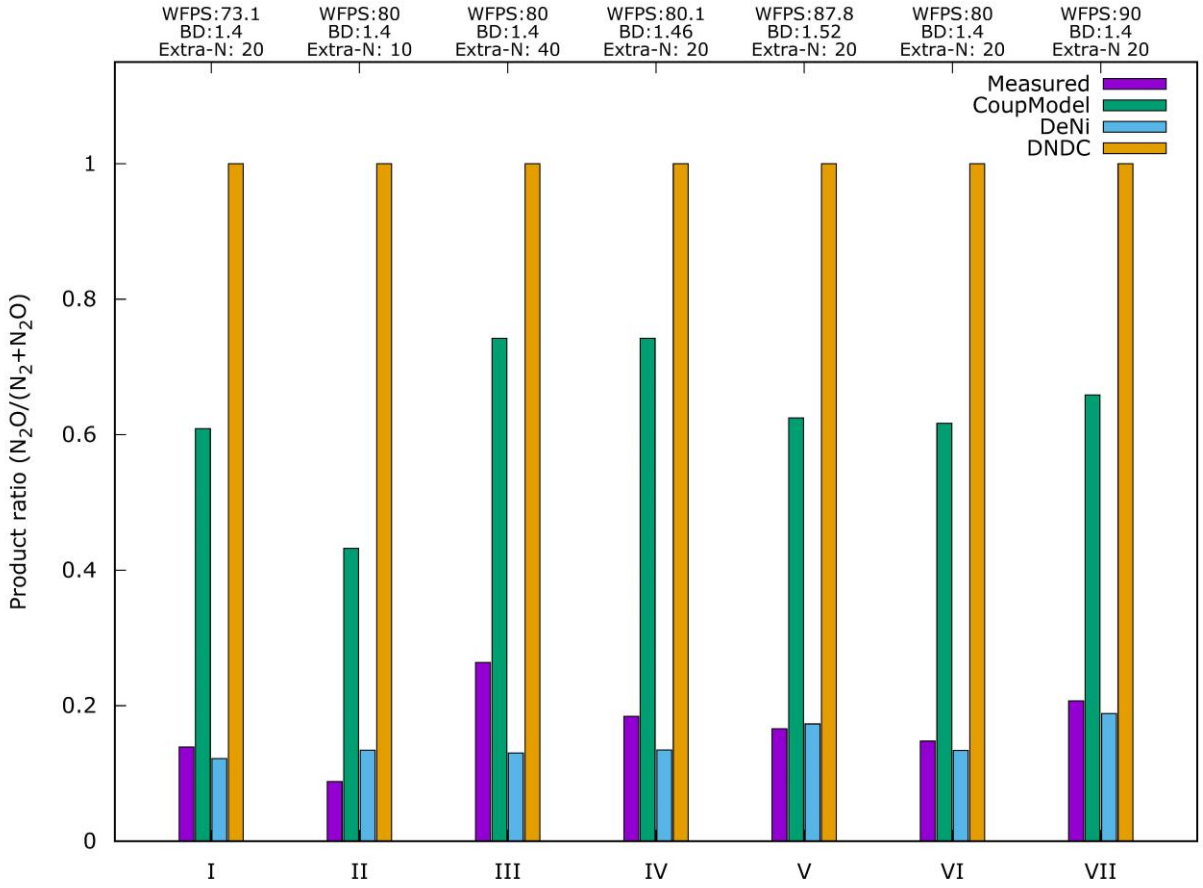

Figure S.6: the $N_2O/(N_2+N_2O)$ ratio of flux measurements during a laboratory incubation of arable, silt-loam arable soil from Hattorf, Germany, compared with modeled fluxes using three biogeochemical models: Coup, DeNi and DNDC.

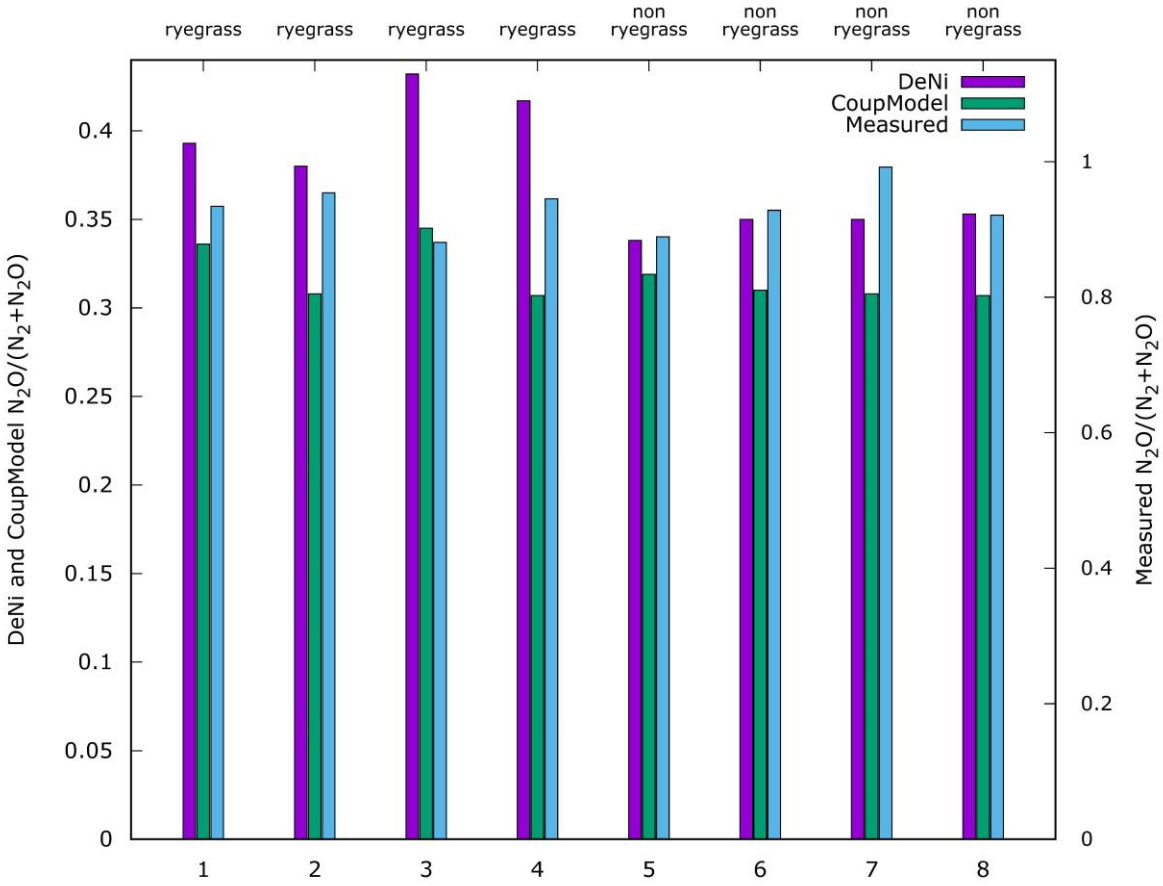

Figure S.7: The product ratio of the DeNi and the CoupModel for the 8 soil columns (4 replicates of 2 treatments: 1-4 with ryegrass, 5-8 control) for sandy arable soil from Fuhrberg, Germany

Table S.4: The ratio of the modelled (DNDC, CoupModel, DeNi) and measured (laboratory incubation) results of N_2 and N_2O fluxes sandy arable soil from Fuhrberg, Germany

	N_2		N_2O		Total denitrification	
	CoupModel	DeNi	CoupModel	DeNi	CoupModel	DeNi
Core 1	0.761	33.23	0.027	1.520	0.076	3.617
Core 2	0.846	24.77	0.018	0.727	0.056	1.824
Core 3	0.198	10.75	0.014	1.106	0.036	2.256

Core 4	0.449	12.92	0.012	0.542	0.036	1.227
Core 5	1.982	74.28	0.116	4.756	0.324	12.50
Core 6	2.515	76.46	0.087	3.189	0.262	8.448
Core 7	30.79	906.2	0.109	3.897	0.353	11.05
Core 8	2.227	65.42	0.085	3.067	0.255	8.010

Table S.5: $N_2O/(N_2 + N_2O)$ ratio of the measured and modeled results of the seven different treatment for silt-loam arable soil from Hattorf, Germany

	Measured	DeNi	CoupModel	DNDC
I	0.139	0.122	0.609	1
II	0.088	0.134	0.432	1
III	0.264	0.130	0.742	1
IV	0.184	0.134	0.742	1
V	0.166	0.173	0.625	1
VI	0.148	0.134	0.617	1
VII	0.207	0.188	0.658	1

Table S.6: 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

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Table S.7: 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 S.8: 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
		Init L1 CN Tot	15.1
		Init L1 Depth	-0.3 m
		Init L1 NTot	20 g/m^2
	Decomposation	RateCoefHumus	0.00041 /day
		RateCoefHumusDis	0.0001 /day
		RateCoefLitter1	0.02 /day
		RateCoefLitter1Dis	0.0005 /day