Evaluation and adjustment of description of denitrification in the CoupModel, DNDC and DeNi model based on N_2 and N_2O laboratory mesocosm incubation system measurements

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Introduction

Denitrification

an anaerobic key process by microbes where the NO_3^- is step-by-step reduced and emitted as NO, N_2O and finally N_2 gas from the soil.

Biogeochemical models

models can be important tools to predict mitigation effects and help to develop climate smart mitigation strategies.

Necessary dataset

data suitable to validate denitrification models are still scarce due to previous technical and/or methodical limitations of measuring N_2 fluxes, but large data-sets are needed in view of the extreme spatio-temporal heterogeneity of denitrification.

Dataset: two mesocosm experiments Hattorf (7 treatments) and Fuhrberg (2 treatments) soils

	Clay	Silt	Sand	Bulk density	NO_3^-	NH_4^+	pH	Total N	Organic C	C/N ratio
	[%]	[%]	[%]	[g/cm^3]	[mg N kg^{-1}]	[mg N kg^{-1}]	(CaCl2)	[%]	[%]	
Fu	3.1	5.9	91.0	1.5	17.8	1.4	4.8	0.1	2.1	15.5
Ha	15.2	77.6	7.2	1.4	12.73	1.27	6	0.1	1.05	10

Table 1: Physical and chemical data of the top soil of the Fuhrberg (5 to 20 cm depth) and Hattorf (0 to 10 cm depth) soils

	Hattorf							Fuhrberg
	I	II	III	IV	V	VI	VII	
Added N (KNO_3) [mg N / kg dry soil]	20	10	40	20	20	20	20	50
atom % ^{15}N in KNO_3	60	98	60	60	60	60	60	60
Thickness of soil layer (cm)	25	25	25	25	25	25	25	10
Bulk density	1.4	1.4	1.4	1.46	1.52	1.4	1.4	1.5
grav. water content	0.25	0.27	0.27	0.25	0.25	0.27	0.30	0.231*
WFPS (%)	73.0	80.0	80.0	80	88	80.0	90.0	80.0*

Table 2: Initial settings of the laboratory experiments (fixed for Fu soil and treatments I to VII of Ha soil)

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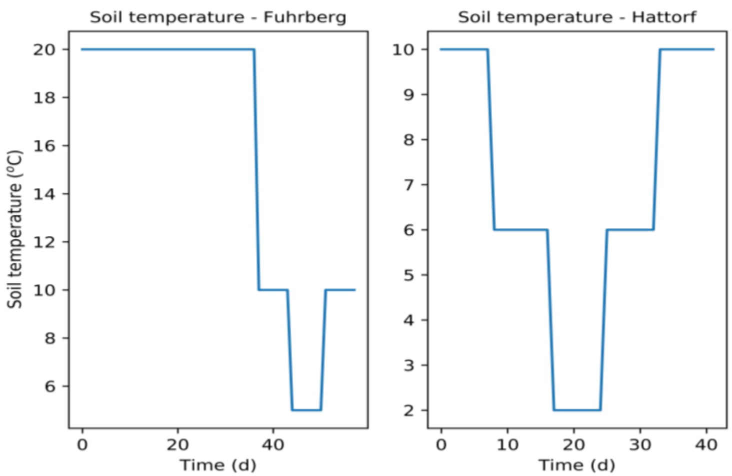

Figure 1: Soil temperature of the mesocosm experiments

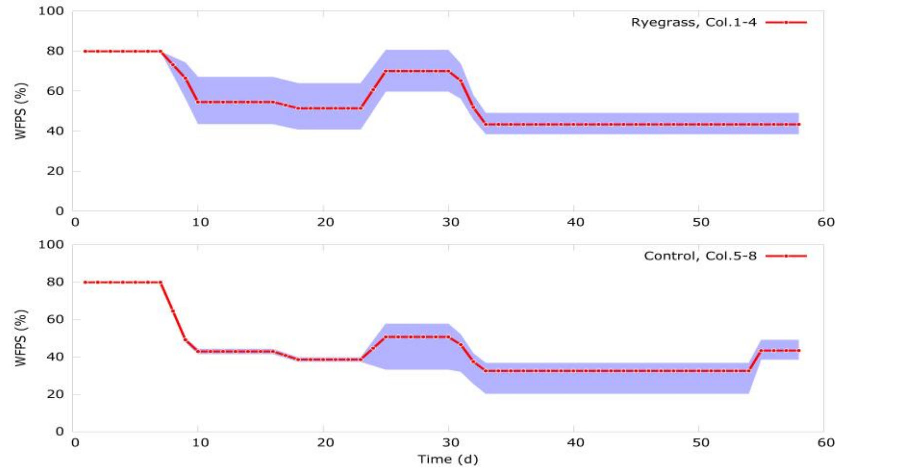

Figure 2: the change of the WFPS of the 8 mesocosm experiments (4 parallel experiment for 2 treatments: C1-4 with and C5-8 without ryegrass) – Furhberg site

Experiment (variants)	NO_3^--N und NH_4^+-N in the unfertilized soil [mg N / kg dry soil]	Added N (KNO_3) [mg N / kg dry soil]	Calculated ^{15}N enrichment (at%) of the NO_3^- in the soil
Ha (II)	14	10	41
Ha (I, IV, V, VI, VII)	14	20	35
Ha (III)	14	40	45
Fu	16	50	60

Table 3: Initial NO_3^--N content, NO_3^--N fertilization and calculated ^{15}N enrichment of NO_3^- after fertilization in the Ha and Fu experiments

Hattorf soil - measured and modeled fluxes

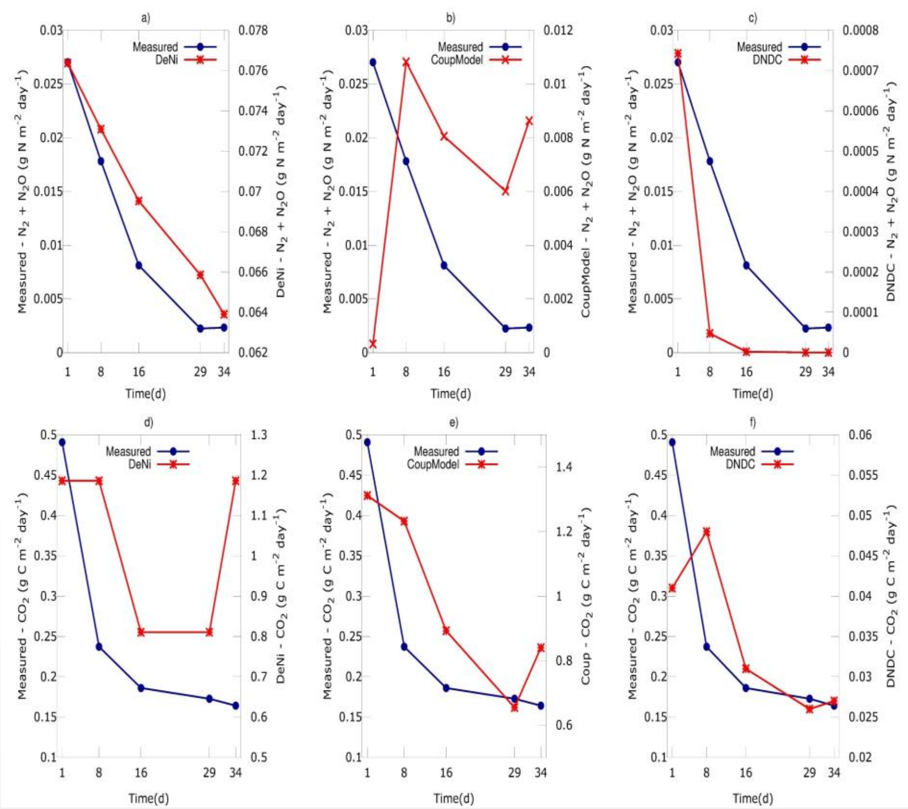

Figure 3: An example for the measured and modeled (DeNi, CoupModel and DNDC) N_2+N_2O (a, b, c) and CO_2 (d,e,f) fluxes of the Ha experiment/$VI_{N20\_80\%\_1.4}$

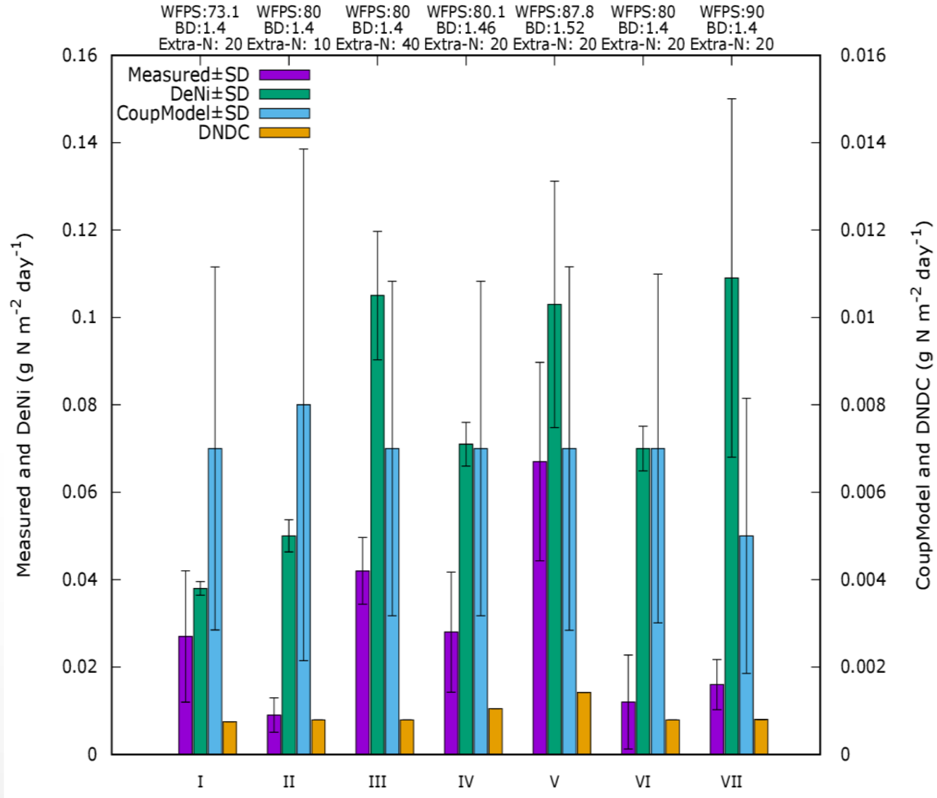

Figure 4: Measured and modeled cumulated N_2+N_2O fluxes of Ha treatments

The changes of the magnitude and the response of the modeled and measured values. The change is equal if the ratio is 1; The modeled values moved from the compared measured values: <0; The modeled values moved to the compared measured values: >0; Ratio calculation (N_2+N_2O) (example): $((I_{Mod}-II_{Mod})/I_{Mod})/((I_{Meas}-II_{Meas})/I_{Meas})$

CoupModel/Measured	$II_{N10\_80\%\_1.4}$	$III_{N40\_80\%\_1.4}$	$IV_{N20\_80\%\_1.46}$	$V_{N20\_88\%\_1.52}$	$VI_{N20\_80\%\_1.4}$	$VII_{N20\_90\%\_1.4}$
$I_{N20\_73\%\_1.4}$	-0.21	0	0	0	0	0.70
$II_{N10\_80\%\_1.4}$	-	-0.03	-0.06	-0.02	-0.38	-0.48
$III_{N40\_80\%\_1.4}$	-	-	0	0	0	0.46
$IV_{N20\_80\%\_1.46}$	-	-	-	0	0	0.67
$V_{N20\_88\%\_1.52}$	-	-	-	-	0	0.38
$VI_{N20\_80\%\_1.4}$	-	-	-	-	-	-0.86
DeNi/Measured	$II_{N10\_80\%\_1.4}$	$III_{N40\_80\%\_1.4}$	$IV_{N20\_80\%\_1.46}$	$V_{N20\_88\%\_1.52}$	$VI_{N20\_80\%\_1.4}$	$VII_{N20\_90\%\_1.4}$
$I_{N20\_73\%\_1.4}$	-0.47	3.17	23.45	1.15	-1.52	-4.59
$II_{N10\_80\%\_1.4}$	-	0.30	0.20	0.16	1.20	1.52
$III_{N40\_80\%\_1.4}$	-	-	0.97	-0.03	0.47	-0.06
$IV_{N20\_80\%\_1.46}$	-	-	-	0.32	0.02	-1.25
$V_{N20\_88\%\_1.52}$	-	-	-	-	0.39	-0.08
$VI_{N20\_80\%\_1.4}$	-	-	-	-	-	1.67
DNDC/Measured	$II_{N10\_80\%\_1.4}$	$III_{N40\_80\%\_1.4}$	$IV_{N20\_80\%\_1.46}$	$V_{N20\_88\%\_1.52}$	$VI_{N20\_80\%\_1.4}$	$VII_{N20\_90\%\_1.4}$
$I_{N20\_73\%\_1.4}$	-0.08	0.10	10.80	0.60	-0.10	-0.16
$II_{N10\_80\%\_1.4}$	-	0	0.16	0.12	0	0.02
$III_{N40\_80\%\_1.4}$	-	-	-0.99	1.34	0	-0.02
$IV_{N20\_80\%\_1.46}$	-	-	-	0.25	0.43	0.56
$V_{N20\_88\%\_1.52}$	-	-	-	-	0.54	0.57
$VI_{N20\_80\%\_1.4}$	-	-	-	-	-	0.04

Fuhrberg soil - measured and modeled fluxes

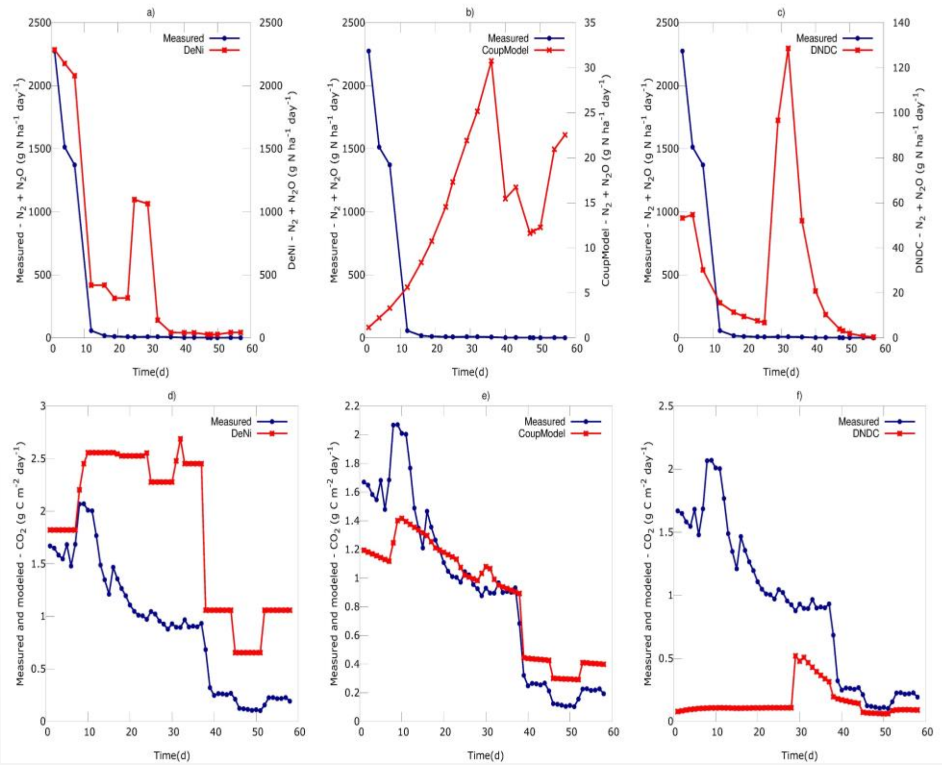

Figure 5: The measured and modeled N_2, N_2O and CO_2 fluxes of the ryegrass treatment of the Fuhrberg soil (Core 1-4)

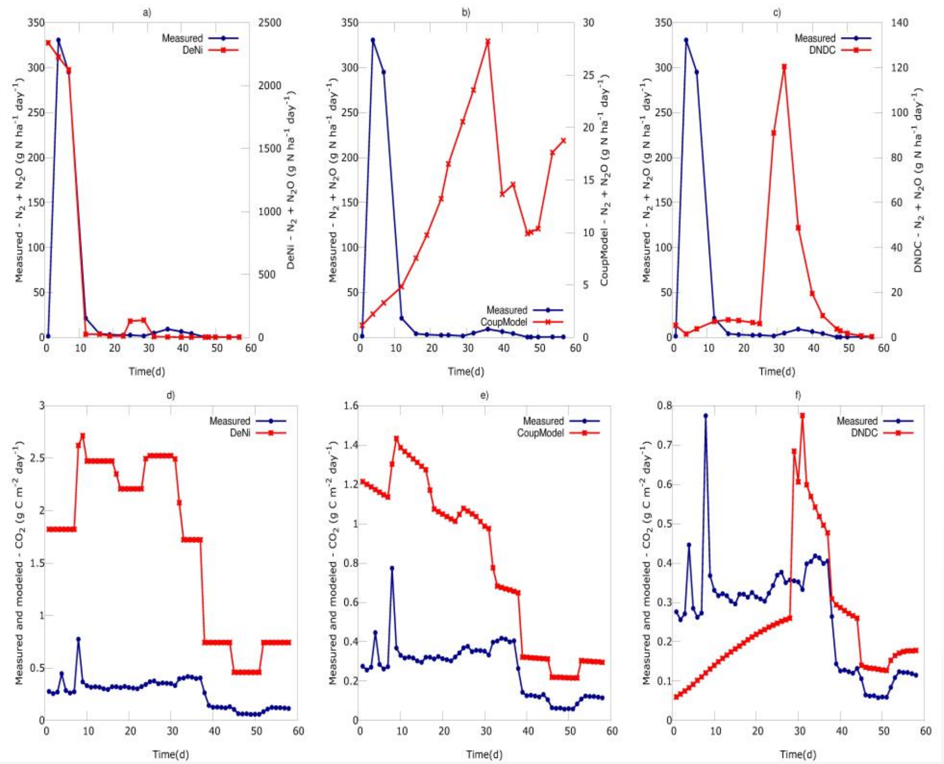

Figure 6: The measured and modeled (DeNi and CoupModel) N_2, N_2O and CO_2 fluxes of the control treatment of the Fuhrberg soil (Core 5-8)

Fuhrberg soil - measured and modeled (CoupModel, DeNi, DNDC) average, cumulative N_2, N_2O and N_2+N_2O, CO_2 fluxes (g N ha^{-1} and g C m^{-2}) and product ratios

		Cores 1-4 (ryegrass)	Cores 5-8 (control)
N_2O	Measured	4818	638.5
	DeNi	4351	2460
	CoupModel	81.90	70.15
	DNDC	507.9	345.4
N_2	Measured	489.8	52.63
	DeNi	6264	4607
	CoupModel	170.7	155.8
	DNDC	0.022	0.019
N_2+N_2O	Measured	5308	691.1
	DeNi	10615	7067
	CoupModel	252.6	226.0
	DNDC	507.9	345.4
$N_2O/(N_2+N_2O)$	Measured	0.9077	0.924
	DeNi	0.410	0.348
	CoupModel	0.324	0.310
	DNDC	0.999	0.999
CO_2	Measured	52.5	15.2
	DeNi	106.1	95.4
	CoupModel	50.848	46.3
	DNDC	8.97	14.14

Conclusion

- The results show that the models did not calculate the same magnitude of the measured values. The DeNi model overestimated and the DNDC and CoupModel underestimated the measured fluxes.

- In several cases the temporal patterns of the measured and the modeled emission were similar.

- The models have limitations in modeling the decomposition of added easily available carbon. Moreover, some processes were missing (e.g. enzymatic effect on the denitrification, modeling of the hot spot effect) or not properly described (e.g. ansvf, product ratio calculation, diffusion).

- The patterns of the modeled values sometimes similar as the measured. It might mean that several processes are described well by the existing models but some parameters should be adjusted and reparametrized based on the new and/or better measurement results and some of the processes are still not represented at the models. The not yet described processes might be the key for the better prediction of the denitrification processes.

Conclusion

- Most cases of over- or underestimations by the models could be explained by certain deficiencies of the models or of the experimental data. The temporal resolution of some experimental data was found to be insufficient for proper model evaluation. Further model evaluation will include testing the DASIM data sets and adjustment of further model parameters.

- The ansvf estimations of the CoupModel were obtained showing that ansvf was almost constant. This is not plausible since the parameters affecting ansvf, i.e. diffusivity and O_2 consumption, must have been highly variable since soil moisture and respiration exhibited large differences between treatments and experimental phases. The underestimation of N_2+N_2O fluxes by CoupModel could therefore result from the inappropriate calculation of ansvf.

Thank you for your attention!