



*Supplement of*

**To what extent can soil moisture and soil Cu contamination stresses affect nitrous species emissions? Estimation through calibration of a nitrification–denitrification model**

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Table S1: Cu in solution (in mgCu. L<sup>-1</sup>) measured at day three of the bioassay experiments performed after each soil initial moisture incubations (expressed in % of the water holding capacity).

Moisture	Cu added total (mgCu.kg soil <sup>-1</sup> )	Cu solution (mg.L <sup>-1</sup> )
30	0	0.024
	50	0.095
	100	0.172
	250	0.32
	500	0.494
	750	0.597
	1000	0.647
	2000	0.641
60	0	0.023
	50	0.113
	100	0.207
	250	0.407
	500	0.606
	750	0.734
	1000	0.784
	2000	0.725
90	0	0.034
	50	0.206
	100	0.206
	250	0.402
	500	0.634
	750	0.502
	1000	0.558
	2000	0.775
DR	0	0.035
	50	0.095
	100	0.162
	250	0.280
	500	0.412
	750	0.440
	1000	0.475
	2000	0.413
DO	0	0.045
	50	0.083
	100	0.155
	250	0.286
	500	0.375
	750	0.443
	1000	0.529
	2000	0.592

Table S2(a): Adj.R2 (Adjusted rsquared) and AIC (Awaik Information Criterion) values for the linear, quadratic and cubic regressions of PNA against added Cu for the bioassays with the various moisture conditions. 30, 60 and 90 are for 30, 60 and 90% Water-Holding Capacity (WHC), DR for Dry-Rewet and DO for Dry-Only. For each moisture condition the bold value corresponds to the model with lowest AIC.

Linear		Quadratic		Cubic		moisture
Adj.R2	AIC	Adj.R2	AIC	Adj.R2	AIC	
0.9206	-71.4824	<b>0.9655</b>	<b>-90.6062</b>	0.9645	-89.0669	30
0.9271	-72.9706	<b>0.9476</b>	<b>-79.9895</b>	0.9452	-78.0966	60
0.9348	-80.4546	0.9339	-79.2689	<b>0.9409</b>	<b>-81.1044</b>	90
<b>0.9303</b>	<b>-101.5814</b>	0.9276	-99.7848	0.9253	-98.1974	DR
0.9238	-89.7099	0.9202	-87.7364	<b>0.9514</b>	<b>-98.8169</b>	DO

Table S2(b): p values of ANOVA between models providing the lowest AIC (Awaik Information Criterion - Table 2a. in bold) for each moisture condition. 30, 60 and 90 are for 30, 60 and 90% of the water holding capacity WHC, DR for Dry-Rewet and DO for Dry-Only. \*For DO incubation, we compared cubic to quadratic rather than cubic to linear because in all other cases, quadratic model was selected.

Moisture condition	ANOVA	
	Compared models	p.value
30	Quadratic cubic	0.541
60	Quadratic cubic	0.768
90	Quadratic cubic	0.077
DR	Quadratic linear	0.6767
DO	Quadratic cubic *	0.001

Table S3: Fitted function for PNA evolution against soil Cu contamination. Results are given for the equations in the form of  $PNA=c+bCu+aCu^2$  with the estimated values of a, b and c and their associated standard errors (SE), for all moisture conditions as well as adjusted r squared. The “60\_90” condition represents the single model that fitted both conditions 60 and 90, further used in the DNDC-Cu model. P.v. = pvalue.

Moisture condition	c	SE c	b	SE b	a	SE a	Adj R2
30	0.78	$1.14 \cdot 10^{-2}$	$-4.49 \cdot 10^{-4}$	$3.53 \cdot 10^{-5}$	$9.49 \cdot 10^{-8}$	$1.74 \cdot 10^{-8}$	0.97
60	0.81	$1.42 \cdot 10^{-2}$	$-4.00 \cdot 10^{-4}$	$4.40 \cdot 10^{-5}$	$6.73 \cdot 10^{-8}$	$2.17 \cdot 10^{-8}$	0.95
90	0.78	$1.44 \cdot 10^{-2}$	$-2.82 \cdot 10^{-4}$	$4.47 \cdot 10^{-5}$	$1.88 \cdot 10^{-8}$	$2.21 \cdot 10^{-8}$	0.93
60_90	0.80	$1.21 \cdot 10^{-2}$	$-3.41 \cdot 10^{-4}$	$3.21 \cdot 10^{-5}$	$4.30 \cdot 10^{-8}$	$1.59 \cdot 10^{-8}$	0.94
	Intercept shift for 90% WHC compared to 60% WHC		SE for intercept shift for 90% WHC compared to 60% WHC		P.v. of intercept shift for 90% WHC compared to 60% WHC		
	$1.29 \cdot 10^{-3}$		$1.23 \cdot 10^{-2}$		0.99		
DR	0.55	$9.41 \cdot 10^{-3}$	$-1.64 \cdot 10^{-4}$	$2.91 \cdot 10^{-5}$	$6.09 \cdot 10^{-9}$	$1.44 \cdot 10^{-8}$	0.93
DO	0.62	$1.21 \cdot 10^{-2}$	$-1.92 \cdot 10^{-4}$	$3.75 \cdot 10^{-5}$	$2.82 \cdot 10^{-9}$	$1.85 \cdot 10^{-8}$	0.92

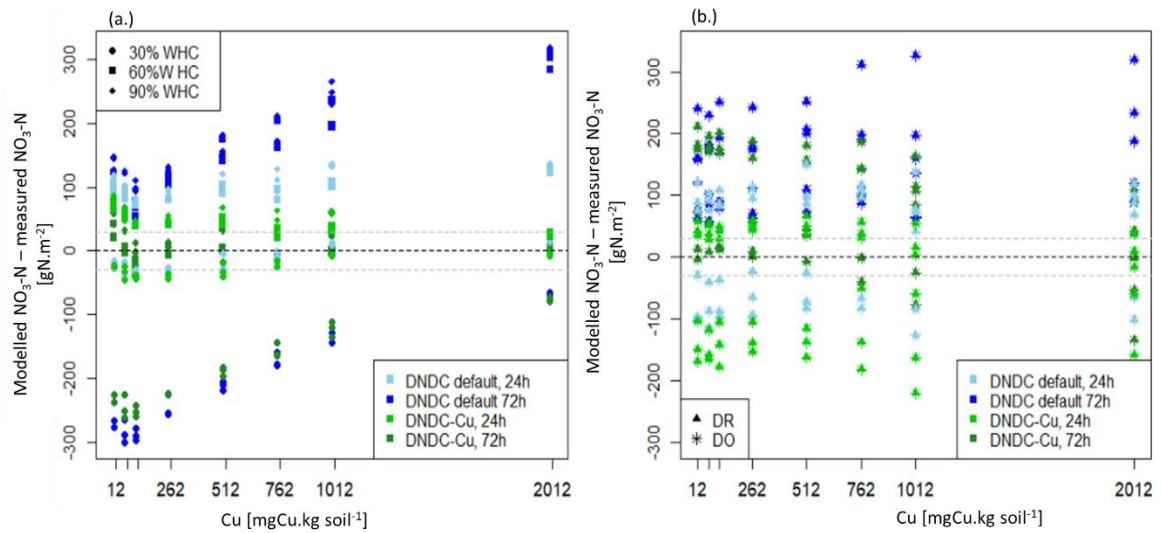


Fig S1: Comparison of modelled and measured soil  $\text{NO}_3\text{-N}$  concentrations using DNDC-Cu and default DNDC versions for the different Cu values used with the five pre-incubations conditions. (a) is for the constant pre-incubation moisture conditions of 30 % of the water holding capacity WHC (circle), 60% WHC (square) and 90% WHC (diamond); (b) is for the pre-incubation at various moisture conditions with Dry-Only (DO, triangle) and Dry-Rewet (DR, star) condition.

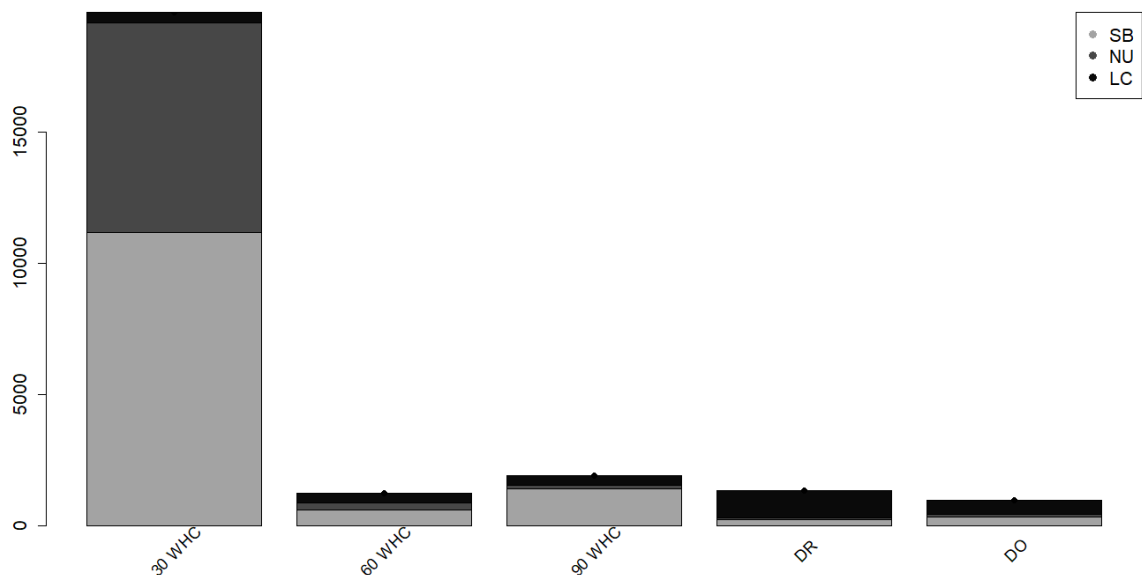


Fig. S2: Mean Standard Deviation decomposition in standard bias (SB), Non-Unity slope (NU) and Lack of Correlation (LC) expressed in  $\text{NO}_3\text{-N}$   $\text{gN.m}^{-2}$  components for the comparison of modelled and measured soil

NO<sub>3</sub>-N. Results are shown for the different moisture incubation conditions (30, 60 and 90% of the WHC (water holding capacity), DR for Dry-Rewet, DO for Dry-Only).

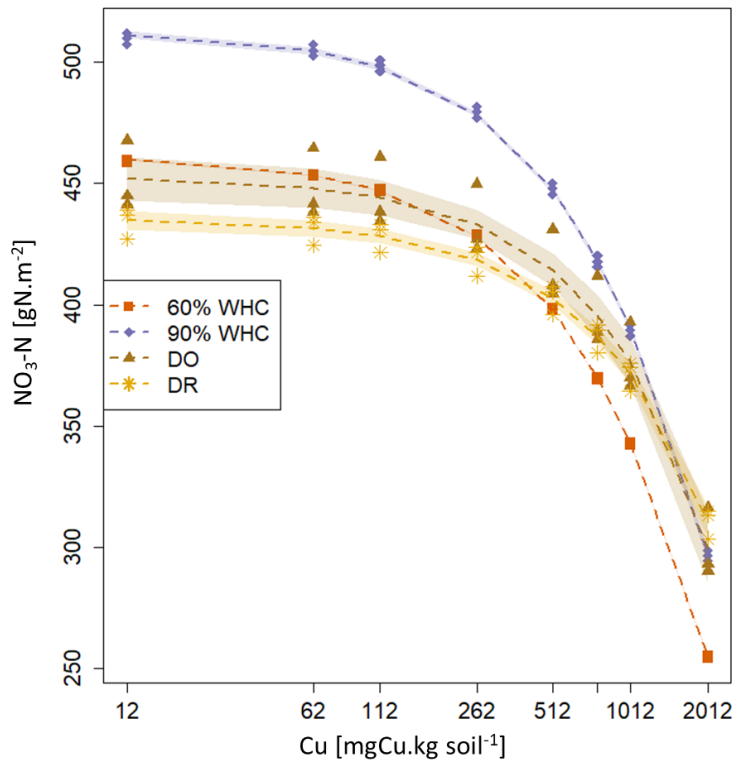


Fig. S3: Predicted soil  $\text{NO}_3\text{-N}$  stocks ( $\text{gN.m}^{-2}$ ) modelled after the 3 days of the bioassay incubation for the four tested soil moisture conditions. Purple diamond is for 90% Water-Holding Capacity (WHC), red square for 60% WHC, brown triangle for Dry-Rewet (DR) and yellow star for Dry-Only (DO). Stocks were modelled for 12, 62, 112, 262, 512, 762, 1012 and 2012  $\text{mg Cu.kg soil}^{-1}$  as represented by pitches, and quadratic fit was used for representation.

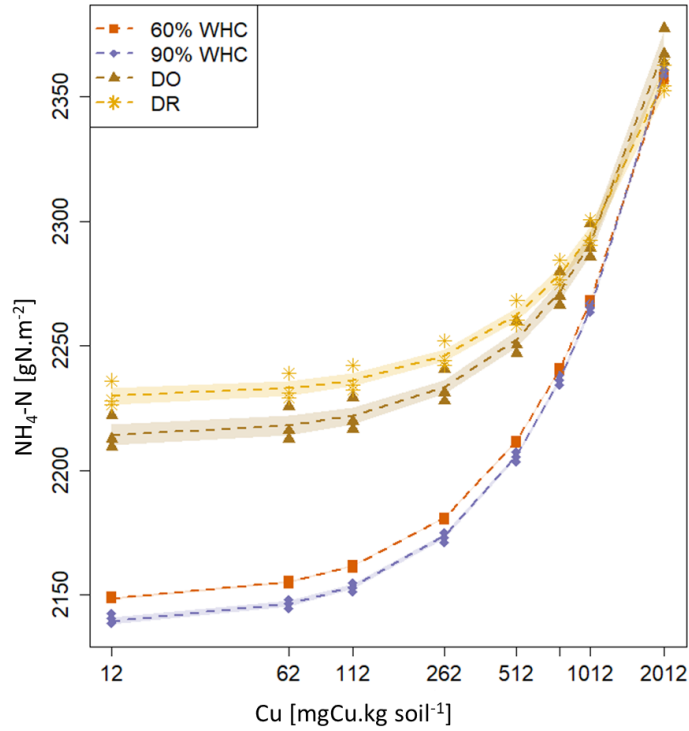


Fig. S4: Soil  $\text{NH}_4\text{-N}$  stocks ( $\text{gN.m}^{-2}$ ) modelled after the 3 days of the bioassay incubation with the four tested soil moisture conditions. Purple diamond is for 90% Water-Holding Capacity (WHC), red square for 60% WHC, yellow star for Dry-Rewet (DR) and brown triangle for Dry-Only (DO). Stocks were modelled for 12, 62, 112, 262, 512, 762, 1012 and 2012  $\text{mg Cu.kg soil}^{-1}$  as represented by pitches, and quadratic fits were used for representation.



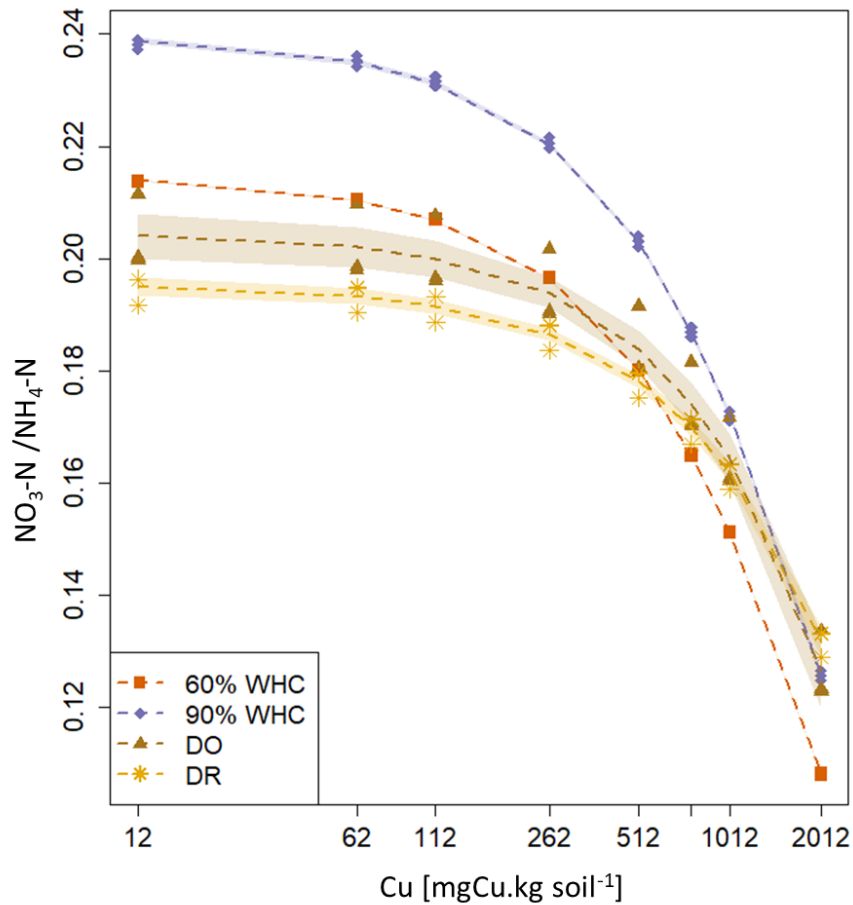


Fig S5: Soil  $\text{NO}_3\text{-N} / \text{NH}_4\text{-N}$  concentrations modelled after the 3 days of the bioassay incubation with the four tested soil moisture conditions. Red square is for 60 % Water-Holding Capacity (WHC), purple diamond is for 90% WHC, yellow star for the Dry-Rewet (DR) and brown triangle for Dry-Only (DO). Soils stocks were modelled for 12, 62, 112, 262, 512, 762, 1012 and 2012  $\text{mg Cu.kg soil}^{-1}$  as represented by pitches, and quadratic fits were used for representation.